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CAS World Wide Web Site (general information)

FILE 'HOME' ENTERED AT 07:51:48 ON 13 JAN 2004

=> fil reg
COST IN U.S. DOLLARS

NEWS WWW

FULL ESTIMATED COST

ENTRY SESSION 0.21

FILE 'REGISTRY' ENTERED AT 07:52:00 ON 13 JAN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 JAN 2004 HIGHEST RN 636558-22-0 DICTIONARY FILE UPDATES: 11 JAN 2004 HIGHEST RN 636558-22-0

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

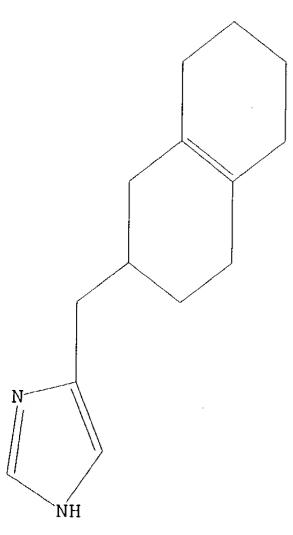
=>
Uploading 09815362g.str

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 07:52:13 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2635 TO ITERATE

38.0% PROCESSED 1000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 49622 TO 55778

PROJECTED ANSWERS:

78 TO 554

L2 6 SEA SSS SAM L1

=> s 11 full

FULL SEARCH INITIATED 07:52:17 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 51880 TO ITERATE

100.0% PROCESSED 51880 ITERATIONS

267 ANSWERS

6 ANSWERS

SEARCH TIME: 00.00.01

L3 267 SEA SSS FUL L1

=> s 13 and caplus/lc

32498121 CAPLUS/LC

· L4 258 L3 AND CAPLUS/LC

=> s 13 not 14

L5 9 L3 NOT L4

=> d 15 1-9

Page 4 01/13/2004

ANSWER 1 OF 9 REGISTRY COPYRIGHT 2004 ACS on STN 337534-09-5 REGISTRY 1H-Imidazole-4-methanol, .alpha.-(6-methoxy-2-naphthalenyl)-.alpha.-propyl-L5 RN CN , (-)- (9CI) (CA INDEX NAME) STEREOSEARCH

MF C18 H20 N2 O2

COM CA CI SR

Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ANSWER 3 OF 9 REGISTRY COPYRIGHT 2004 ACS on STN 336102-60-4 REGISTRY

Acetamide, N-[6-[1-hydroxy-1-(lH-imidazol-4-yl)-2-methylpropyl]-2-naphthalenyl]-, (+)- (9CI) (CA INDEX NAME)
STEREOSEARCH
C19 H21 N3 O2

FS

MF

CICOM

Rotation (+).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ANSWER 2 OF 9 REGISTRY COPYRIGHT 2004 ACS on STN

336103-05-0 REGISTRY

2-Naphthalenecarboxamide, 6-[(1S)-1-hydroxy-1-(lH-imidazol-4-yl)-3-CN

methylbutyl]-N-methyl- (9CI) (CA INDEX NAME)
STEREOSEARCH

C20 H23 N3 O2 MF

CI COM

SR CA

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ANSWER 4 OF 9 REGISTRY COPYRIGHT 2004 ACS on STN

336102-58-0 REGISTRY

1H-Imidazole-4-methanol, .alpha.-(6-ethoxy-2-naphthalenyl)-.alpha.-(1-methylethyl)-, (-)- (9CI) {CA INDEX NAME} STEREOSEARCH CN

C19 H22 N2 O2 MF

COM SR CA

Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Page 5 01/13/2004

RN

ANSWER 5 OF 9 REGISTRY COFYRIGHT 2004 ACS on STN 247173-10-0 REGISTRY 1H-Imidazole-4-methanol, .alpha.-(1,1-dimethylethyl)-.alpha.-(6-methoxy-2-CNnaphthalenyl) - (9C1) (CA INDEX NAME)

3D CONCORD

C19 H22 N2 O2

COM SR CA

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ANSWER 7 OF 9 REGISTRY COPYRIGHT 2004 ACS ON STN 150560-49-9 REGISTRY

Acetic acid, [[6-[[2-(diphenylmethyl)-1H-imidazol-4-yl]methyl]-5,6,7,8-tetrahydro-1-naphthalenyl]oxy)-, methyl ester (9CI) (CA INDEX NAME)

3D CONCORD

MF SR C30 H30 N2 Q3 CA

$$CH_2 \xrightarrow{H} CHPh_2$$

$$MeO-C-CH_2-O$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ANSWER 6 OF 9 REGISTRY COPYRIGHT 2004 ACS on STN

247173-08-6 REGISTRY

CN 1H-Imidazole-4-methanol, .alpha.-cyclopropyl-.alpha.-(6-methoxy-2naphthalenyl) - (9CI) (CA INDEX NAME) 3D CONCORD

MF C18 H18 N2 Q2

CI COM

SR CA

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ANSWER 8 OF 9 REGISTRY COPYRIGHT 2004 ACS on STN

75601-48-8 REGISTRY Methanone, 1H-imidazol-4-y1[4b,5,6,7,8,8a,9,10-octahydro-4b,8-dimethy1-2-(1-methylethyl)-9-phenanthrenyl]-, {4bS-(4b.alpha.,8.alpha.,8a.beta.)}-(9CI) (CA INDEX NAME) STEREOSEARCH

C23 H30 N2 O STN Files: BEILSTEIN*, SPECINFO (*File contains numerically searchable property data)

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Page 6 01/13/2004

L5 ANSWER 9 OF 9 REGISTRY COPYRIGHT 2004 ACS on STN
RN 75601-29-5 REGISTRY
CN Methanone, [4b,5,6,7,9,10-hexahydro-4b,8-dimethy1-2-(1-methylethy1)-9phenanthrenyl]-lH-imidazol-4-yl-, (4bS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H28 N2 O

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

=> fil caplus
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 176.20 176.41

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FILE COVERS 1907 - 13 Jan 2004 VOL 140 ISS 3 FILE LAST UPDATED: 12 Jan 2004 (20040112/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 14 L6 33 L4

=> d ibib abs hitstr 1-33

Page 8 01/13/2004

L6 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

2003:951005 CAPLUS ACCESSION NUMBER:

140:5050 DOCUMENT NUMBER:

Preparation of 4-substituted imidazole-2-thiones and TITLE: imidazol-2-ones as agonists of alpha-2B and alpha-2C adrenergic receptors

INVENTOR(S): Chow, Ken; Heidelbaugh, Todd: Gil, Daniel: Garst,

Michael: Wheeler, Larry A.; Nguyen, Phong X.; Gomez, Bario G.

PATENT ASSIGNEE(S): Allergan, Inc., USA

PCT Int. Appl., 163 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

> PATENT NO. KIND DATE APPLICATION NO. DATE WO 2003099795 A1 20031204 WO 2003-US15441 20030516 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, EE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ. GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-153328 A 20020521

The title compds. [I; Y in the ring is optional and represents a heteroatom selected from N, O and S with the proviso that the N atom is trivalent, and the O or S atoms are divalent; m = 0, 1; n, p = 0, 1, 2; X= 0, S; the dashed lines represent a bond, or absence of bond with the proviso that only one double bond is present in the ring and that two adjoining dashed lines do not both represent a bond; R1-R4 = independently H, (un)substituted Ph, C1-4 alkyl, C3-5 cycloalkyl, CH2CN, CH2SR5, CH2NR6R6, COR5, CH2OR5, OR6, SR6, NR6R6, C2-4 alkenyl or alkynyl, F, C1, Br, iodo, CF3, cyano, an oxygen double bonded to the ring carbon with the proviso that the adjacent dashed line within the ring represents absence of a bond; R5 = H, OR7, C1-4 alkyl, CF3, C3-6 cycloalkyl, (un) substituted

ANSWER 1 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

628732-25-2 CAPLUS

Acetonitrile, [3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-1(2H)-

naphthalenylidene]-, (22)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

628730-35-8P 628730-36-9P

RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 4-substituted imidazolethiones and imidazolones as agonists of .alpha.2B and .alpha.2C adrenergic receptors)

628730-35-8 CAPLUS

1(2H)-Naphthalenone, 2-[(2,3-dihydro-2-thioxo-1H-imidazol-4-v1)methyl]-3,4-

dihydro-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

628730-36-9 CAPLUS

1(2H)-Naphthalenone, 2-[(2,3-dihydro-2-thioxo-1H-imidazol-4-yl)methyl]-3,4dihydro-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

ANSWER 1 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN Ph or 5 or 6 membered heteroaryl having 1 to 3 heteroatoms selected from O, S, and N: R6 = H, C1-4 alkyl, allyl, C3-6 cycloalkyl, (un)substituted Ph or 5 or 6 membered heteroaryl having 1 to 3 heteroatoms selected from 0, 5, and N; R7 = H, C1-4 alkyl, allyl, C3-6 cycloalkyl, (un) substituted phenyl; R1 and R2 or R2 and R3 or R3 and R4 together can form a ring together with the resp. carbons to which each of these is attached; R10 \Rightarrow H, Cl-6 or alkyl] are prepd. These compds. possess specific or selective binding activity to .alpha.2B and/or .alpha.2C adrenergic receptors in preference over .alpha.A adrenergic receptors, and as such have no or only minimal cardiovascular and/or sedative activity. They are useful as medicaments in mammals, including humans, for treatment of diseases and or alleviation of conditions which are responsive to treatment by agonists of .alpha.B adrenergic receptors. The diseases and conditions include pain, allodynia, chronic pain, visceral pain, neuropathic pain, corneal pain, glaucoma, elevated intraocular pressure, ischemic neuropathies, neurodegenerative diseases, diarrhea, nasal congestion, muscle spasticity, diuresis, withdrawal syndromes, optic neuropathy, spinal ischemia, stroke, memory and cognition deficits, attention deficit disorder, psychoses, manic disorders, anxiety, depression, hypertension, congestive heart failure, cardiac ischemia, arthritis, spondylitis, gouty arthritis, osteoarthritis, juvenile arthritis, autoimmune diseases, lupus erythematosus, chronic gastrointestinal inflammations, Crohn's disease, gastritis, irritable bowel disease (IBD), functional dyspepsia and ulcerative colitis. For example, 4-(4-methylindan-2-yl)-1,3-dihydroimidazole-2-thione showed agonism activity on .alpha.2B and alpha.2C adrenergic receptors with EC50 of 3 and 13 nM, resp. and no

activity on .alpha.2A adrenergic receptor. 157058-52-1P 628732-24-1P 628732-25-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of 4-substituted imidazolethiones and imidazolones as agonists of .alpha.2B and .alpha.2C adrenergic

receptors) 157058-52-1 CAPLUS

 $lH-Imidazole, \ 4-[\{1,2,3,4-tetrahydro-2-naphthalenyl\}]-\ (9CI) \ \ (CA)$

629732-24-1 CAPLUS

Double bond geometry as shown.

Acetonitrile, [3,4-dihydro-2-(lH-imidazol-4-ylmethyl)-1(2H)-

naphthalenylidene]-, {2E}- (9CI) (CA INDEX NAME)

ANSWER 1 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

423773-40-4P 628730-38-1P 628730-40-5P 628730-44-9P 628730-45-0P 628730-46-1P 628730-47-2P 628730-48-3P 628730-49-4P 628730-50-7P 628730-51-8P 628730-52-9P 628730-53-0P 628730-88-1P 628731-16-8P 628731-17-9P 628731-32-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(prepn. of 4-substituted imidazolethiones and imidazolones as agonists of .alpha.2B and .alpha.2C adrenergic receptors)

423773-40-4 CAPLUS

1(2H) -Naphthalenone, 2-[(2,3-dihydro-2-thioxo-1H-imidazol-4-yl)methyl]-3,4dihydro- (9CI) (CA INDEX NAME)

628730-38-1 CAPLUS

1(2H) -Naphthalenone, 2-[(2,3-dihydro-2-thioxo-1H-imidazol-4-yl)methyl]-3,4dihydro-4-methyl- (9CI) (CA INDEX NAME)

628730-40-5 CAPLUS

1(2H)-Naphthalenone, 2-[{2,3-dihydro-2-thioxo-1H-imidazol-4-yl}methyl]-3,4dihydro-6-hydroxy- (9CI) (CA INDEX NAME)

628730-44-9 CAPLUS

2H-Imidazole-2-thione, 1,3-dihydro-4-{(1,2,3,4-tetrahydro-2naphthalenyl) methyl - (9CI) (CA INDEX NAME)

Page 9 01/13/2004

L6 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 628730-45-0 CAPLUS
CN 2H-Imidazole-2-thione, 1,3-dihydro-4-[[(2S)-1,2,3,4-tetrahydro-2-naphthalenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 628730-46-1 CAPLUS

CN 2H-Imidazole-Z-thione, 1,3-dihydro-4-[[{2R}]-1,2,3,4-tetrahydro-2-naphthalenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 628730-47-2 CAPLUS

Il (2H) -Naphthalenone, 2-[(2,3-dihydro-2-thioxo-1H-imidazol-4-yl)methyl] - 3,4,5,6,7,8-hexahydro- (9CI) (CA INDEX NAME)

RN 628730-48-3 CAPLUS

V 2H-Imidazole-2-thione, 1,3-dihydro-4-[(1,2,3,4,5,6,7,8-octahydro-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

L6 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

$$CH_2$$
 H
 S

RN 628730-53-0 CAPLUS

N 1(2H)-Naphthalenone, 2-{(2,3-dihydro-2-thioxo-1H-imidazol-4-yl)methyl}-6-fluoro-3,4-dihydro- (9CI) (CA INDEX NAME)

CH2 H

RN 628730-88-1 CAPLUS

CN 1(2H)-Naphthalenone, 8-chloro-2-[(2,3-dihydro-2-thioxo-1H-imidazol-4-

yl)methyl]-3,4-dihydro- (9CI) (CA INDEX NAME)

RN 628731-16-8 CAPLUS

CN Acetonitrile, [2-[(2,3-dihydro-2-thioxo-lH-imidazol-4-yl)methyl]-3,4-dihydro-1(2H)-naphthalenylidene]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 628731-17-9 CAPLUS

CN Acetonitrile, [2-[(2,3-dihydro-2-thioxo-1H-imidazol-4-yl)methyl]-3,4-dihydro-1(2H)-naphthalenylidene]-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L6 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Contin

RN 628730-49-4 CAPLUS

CN 2H-Imidazole-2-thione, 1,3-dihydro-4-[[(2R)-1,2,3,4,5,6,7,8-octahydro-2-naphthalenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 628730-50-7 CAPLUS

CN 1(2H)-Naphthalenone, 2-[(2,3-dihydro-2-thioxo-1H-imidazol-4-yl)methyl]-3,4-dihydro-8-(hydroxymethyl)- (9Cl) (CA INDEX NAME)

RN 628730-51-8 CAPLUS

CN 1(2H)-Naphthalenone, 2-[(2,3-dihydro-2-thioxo-lH-imidazol-4-yl)methyl]-3,4-dihydro-8-methyl- (9CI) (CA INDEX NAME)

RN 628730-52-9 CAPLUS

CN 1(2H)-Naphthalenone, 2-[(2,3-dihydro-2-thioxo-1H-imidazol-4-yl)methyl]-8-fluoro-3,4-dihydro-(9CI) (CA INDEX NAME)

L6 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 628731-32-8 CAPLUS

CN 2H-Imidazol-2-one, 1,3-dihydro-4-{(1,2,3,4-tetrahydro-1-oxo-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

IT 226571-13-7P

RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREF (Preparation); RACT (Reactant or reagent) (preps. of 4-substituted imidazolethiones and imidazolones as agonists

of .alpha.2B and .alpha.2C adrenergic receptors)
RN 226571-13-7 CAPLUS

CN 1H-Imidazole, 4-[[(2S)-1,2,3,4-tetrahydro-2-naphthalenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 157058-44-1P 226571-02-4P 226571-05-7P

RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)

(prepn. of 4-substituted imidazolethiones and imidazolones as agonists

of .alpha.2B and .alpha.2C adrenergic receptors)

CN 1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)- (9CI) (CA INDEX NAME)

RN 226571-02-4 CAPLUS

Page 10 01/13/2004

ANSWER 1 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) 1(2H)-Naphthalenone, 3,4,5,6,7,8-hexahydro-2-(1H-imidazol-4-ylmethyl)-(9CI) (CA INDEX NAME)

226571-05-7 CAPLUS 1H-Imidazole, 4-[(1,2,3,4,5,6,7,8-octahydro-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

ΙT 628731-55-5

RL: RCT (Reactant); RACT (Reactant or reagent) (reactant; prepn. of 4-substituted imidazolethiones and imidazolones as agonists of .alpha.2B and .alpha.2C adrenergic receptors) 628731-55-5 CAPLUS

1H-Imidazole, 4-[[(2R)-1,2,3,4,5,6,7,8-octahydro-2-naphthalenyl]methyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\bigcap_{\mathbf{R}} \bigcap_{\mathbf{N}} \bigcap_{\mathbf{N}}$$

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

628730-35-8 CAPLUS

1(2H)-Naphthalenone, 2-[(2,3-dihydro-2-thioxo-1H-imidazol-4-yl)methyl]-3,4-dihydro-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

628730-36-9 CAPLUS

1(2H)-Naphthalenone, 2-[(2,3-dihydro-2-thioxo-1H-imidazol-4-yl)methyl]-3,4dihydro-, (2R) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

ANSWER 2 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:950846 CAPLUS

DOCUMENT NUMBER: 140:13072

TITLE: Novel methods and compositions for alleviating pain

INVENTOR(S): Gil, Daniel W.: Donello, John E. PATENT ASSIGNEE(S):

Allergan, Inc., USA PCT Int. Appl., 129 pp. CODEN: PIXXD2 SOURCE:

DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PR

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG US 2003229088 A1 20031211 US 2002-153154 20020521 RITY APPLN. INFO.:	WO	2003	0992	89	Α	2	2003	1204		W	20	03-ช	s130	57	2003	0423		
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AB at least three days, such that relief of chronic pain is maintained in the absence of continued activation of said receptor. The analgesic

.alpha.-adrenergic receptor can be, for example, the .alpha.-2B receptor. 423773-40-4 423773-40-4D, stereoisomers

628730-35-8 628730-36-9

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses) (.alpha.-adrenoceptor activation for alleviating pain)

423773-40-4 CAPLUS

1(2H)-Naphthalenone, 2-[(2,3-dihydro-2-thioxo-1H-imidazol-4-yl)methyl]-3,4dihydro- (9CI) (CA INDEX NAME)

423773-40-4 CAPLUS

1(2H)-Naphthalenone, 2-[(2,3-dihydro-2-thioxo-1H-imidazol-4-yl)methyl]-3,4-dihydro-(9CI) (CA INDEX NAME)

L6 ANSWER 3 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

2003:77587 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 138:122649

TITLE: Preparation of imidazoles as selective agonists at .alpha.2B or .alpha.2B/.alpha.2C adrenergic receptors INVENTOR(S): Chow, Ken; Gil, Daniel W.: Burke, James A.; Harcourt,

Dale A.; Garst, Michael E.; Wheeler, Larry A. PATENT ASSIGNEE (S):

Allergan Sales, Inc., USA
U.S. Pat. Appl. Publ., 53 pp., Cont.-in-part of U.S.
Ser. No. 329,752, abandoned. SOURCE:

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC, NUM. COUNT: PATENT INFORMATION:

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		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,		
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OTHER SOURCE(S):

Title compds. I [x = 1-2; R1 = H, halo, alk(en/yn)yl, etc.; R2-3 = H, halo, alk(en/yn)yl, etc.] which are selective agonists at .alpha.2B or .alpha.2B/.alpha.2C adrenergic receptors and useful for the treatment of conditions including pain, particularly chronic pain, glaucoma or elevated

MARPAT 138:122649

Page 11 01/13/2004

ANSWER 3 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN intraocular pressure with reduced cardiovascular or sedative side effects, are claimed. Also included are methods of making and using such compds. Intrinsic activities towards .alpha.2A, .alpha.2B, .alpha.2C adrenergic receptors of .apprx.100 of the claimed compds. relative to

brimonidine/oxymetazoline are tabulated. 157058-47-4P, 1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-7-methoxy-RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation): RACT (Reactant or reagent): USES (Uses) (prepn. of imidazoles as selective agonists at .alpha.2b or .alpha.2b/.alpha.2c adrenergic receptors) 157058-47-4 CAPLUS

1(2H) -Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl) -7-methoxy-(9CI) (CA INDEX NAME)

IT 157058-44-1P, 1 (2H) -Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl) - 157058-52-1P, 1H-Imidazole, 4-[(1,2,3,4-tetrahydro-2naphthalenyl) methyl] - 157058-55-4P, IH-Imidazole, 4-[(1,2,3,4-tetrahydro-7-methoxy-2-naphthalenyl)methyl]-226570-89-4P, 1H-Imidazole, 4-{(1,2,3,4-tetrahydro-7-methoxy-2naphthalenyl)methyl]-, monohydrochloride 226571-02-4P, 1(2H)-Naphthalenone, 3,4,5,6,7,8-hexahydro-2-(1H-imidazol-4-ylmethyl)-226571-05-7P, 1H-Imidazole, 4-[(1,2,3,4,5,6,7,8-octahydro-2-naphthalenyl)methyl]-226571-13-7P, 1H-Imidazole, 4-[[(2S)-1,2,3,4-tetrahydro-2-naphthalenyl]methyl]- 226571-14-8P , lH-Imidazole, 4-[[(2R)-1,2,3,4-tetrahydro-2-naphthalenyl]methyl]-226571-25-1P, lH-Imidazole, 4-[(1,2,3,4-tetrahydro-4-methyl-2-naphthalenyl)methyl]-226571-26-2P, l(2H)-Naphthalenone, 3,4-dihydro-2-(lH-imidazol-4-ylmethyl)-4-methyl-226571-35-3P, 1H-Imidazole, 4-[(1,2,3,4-tetrahydro-4,4-dimethyl-2-naphthalenyl)methyl]-226571-36-4P, 1H-Imidazole, 4-[(1,2,3,4-tetrahydro-7-methyl-2naphthalenyl) methyl]-, monohydrochloride 226571-37-5P, 1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-7-methyl-RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(prepn. of imidazoles as selective agonists at .alpha.2b or alpha.2b/.alpha.2c adrenergic receptors)

157058-44-1 CAPLUS

1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)- (9CI) (CA

ANSWER 3 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

$$CH_2$$

226571-05-7 CAPLUS CN lH-Imidazole, 4-[(1,2,3,4,5,6,7,8-octahydro-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

1H-Imidazole, 4-[[(2S)-1,2,3,4-tetrahydro-2-naphthalenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

226571-14-8 CAPLUS 1H-Imidazole, 4-[[(2R)-1,2,3,4-tetrahydro-2-naphthalenyl]methyl]+ (9CI) (CA INDEX NAME)

Absolute stereochemistry.

1H-Imidazole, 4-[(1,2,3,4-tetrahydro-4-methyl+2-naphthalenyl)methyl]-(9CI) (CA INDEX NAME)

ANSWER 3 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

157058-52-1 CAPLUS

CN 1H-Imidazole, 4-[(1,2,3,4-tetrahydro-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

157058-55-4 CAPLUS

1H-Imidazole, 4-{(1,2,3,4-tetrahydro-7-methoxy-2-naphthalenyl)methyl]-(9CI) (CA INDEX NAME) CN

226570-89-4 CAPLUS

lH-Imidazole, 4-[(1,2,3,4-tetrahydro-7-methoxy-2-naphthalenyl)methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\mathsf{Me0} \qquad \qquad \mathsf{CH}_2 \qquad \mathsf{N} \qquad \mathsf{N}$$

HC1

226571-02-4 CAPLUS

1(2H)-Naphthalenone, 3,4,5,6,7,8-hexahydro-2-(1H-imidazol-4-ylmethyl)-(9CI) (CA INDEX NAME)

ANSWER 3 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

(Continued)

226571-26-2 CAPLUS

1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-4-methyl-(9CI) (CA INDEX NAME)

226571-35-3 CAPLUS

 $1 \\ H-Imidazole, \ 4-\{(1,2,3,4-tetrahydro-4,4-dimethyl-2-naphthalenyl)\ methyl\}-1 \\ H-Imidazole, \ 4-\{(1,2,3,4-tetrahydro-4,4-dimethyl-2-naphthalenyl)\ methyl]-1 \\ H-Imidazole, \ 4-\{(1,2,3,4-tetrahydro-4,4-dimethyl-2-naphthalenyl)\ methylland \ 4-\{(1,2,3,4-tet$ (9CI) (CA INDEX NAME)

RN 226571-36-4 CAPLUS

1H-Imidazole, 4-[(1,2,3,4-tetrahydro-7-methyl-2-naphthalenyl)methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Me
$$CH_2$$
 N

HC1

226571-37-5 CAPLUS

1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-7-methyl-CN (9CI) (CA INDEX NAME)

226571-57-9P, 1-Naphthalenol, 1,2,3,4-tetrahydro-2-(1H-imidazol-4-17 ylmethyl)-7-methoxy-RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

Page 12 01/13/2004

ANSWER 3 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) (prepn. of imidazoles as selective agonists at .alpha.2b or .alpha.2b/.alpha.2c adrenergic receptors)

226571-57-9 CAPLUS 1-Naphthalenol, 1,2,3,4-tetrahydro-2-(1H-imidazol-4-ylmethyl)-7-methoxy-(9CI) (CA INDEX NAME)

ANSWER 4 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) In I, each x is independently 1 or 2; each R1 is independently H; halogen; C1-4 alkyl; C1-4 alkynyl; -COR4 where R4 is H, C1-4 alkyl or C1-4 alkoxy; C3-6 cycloalkyl; aryl; heteroaryl; cyano; nitro; trihalomethyl; oxo; or -(CH2)n-X-(CH2)m-(R5)o where X is O, S or N, n is 0-3, m is 0-3, o is 0-1, and R5 is Me or H1-2. Each R2 and each R3 are independently H; halogen; C1-4 alkyl; C1-4 alkenyl; C1-4 alkynyl; -COR4 where R4 is H; C1-4 alkyl or C1-4 alkoxy; C3-6 cycloalkyl; aryl; heteroaryl; cyano; nitro; trihalomethyl; oxo; or -(CH2)n-X-(CH2)m-(R5)o where X is O, S or N, n is 0-3, m is 0-3, o is 0-1, and R5 is Me or H1-2; or an R2 and an R3 together condense to form and the markly start. or an R2 and an R3 together condense to form a satd., partly satd., or unsatd. ring structure having the formula -[C(R6)p]q-Xs-[C(R6)p]r-Xt-[C(R6)p]u where each R6 is independently H; halogen; C1-4 alkyl; C1-4 alkenyl; C1-4 alkynyl; -COR4 where R4 is H, C1-4 alkyl or C1-4 alkoxy; C3-6 cycloalkyl; aryl; heteroaryl; cyano; nitro; trihalomethyl and oxo where each p is independently 1 or 2, q is 0-5, r is 0-5, u is 0-5. Each X is independently 0, S, or N and s is 0 or 1; provided that q+r+u+s+t<6. Y is 0, S; N; -[C(R7)z]s-, where each R7 is independently as previously defined for R1, each z is independently 1-2, and s is 1-3; -CH: , -CH:CH-; or Y1CH2, where Y1 is 0, N, or S; and the dotted lines in I are optional double bonds, with the proviso that if the ring including Y is a cyclohexane ring or a heterocyclic 5 member ring said ring is not fully unsatd., and that if Y is O, N or S, the ring including Y contains at least one said double bond. Intrinsic activities towards .alpha.2A, .alpha.2B, .alpha.2C adrenergic receptors of .apprx.100 of the claimed relative to brimonidine/охуmetazoline are tabulated. Although the methods of prepn. are not claimed, .apprx.100 example prepns. are included.

157058-47-4P, 1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4ylmethyl) -7-methoxy-

RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation): THU (Therapeutic use): BIOL (Biological study): PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of imidazoles as selective agonists at .alpha.2b or

.alpha.2b/.alpha.2c adrenergic receptors) 157050-47-4 CAPLUS

1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-7-methoxy-(9CI) (CA INDEX NAME)

157058-44-1P, 1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4ylmethyl) - 157058-52-1P, 1H-Imidazole, 4-[(1,2,3,4-tetrahydro-2naphthalenyl) methyl] - 157058-55-4P, lH-Imidazole, 4-[(1,2,3,4-tetrahydro-7-methoxy-2-naphthalenyl)methyl] 226570-89-4P, 1H-Imidazole, 4-[(1,2,3,4-tetrahydro-7-methoxy-2naphthalenyl) methyl] -, monohydrochloride 226571-02-4P, 1(2H)-Naphthalenone, 3,4,5,6,7,8-hexahydro-2-(1H-imidazol-4-ylmethyl) -226571-05-7P, 1H-Imidazole, 4-[(1,2,3,4,5,6,7,8-octahydro-2naphthalenyl) methyl) - 226571-13-7P, 1H-Imidazole, 4-[[(2S)-1,2,3,4-tetrahydro-2-naphthalenyl]methyl]- 226571-14-8P , lH-Imidazole, 4-[[(2R)-1,2,3,4-tetrahydro-2-naphthalenyl]methyl]-226571-25-1P, 1H-Imidazole, 4-{(1,2,3,4-tetrahydro-4-methyl-2-naphthalenyl) methyl}- 226571-25-2P, 1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-4-methyl- 226571-35-3P,

ANSWER 4 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:754359 CAPLUS

DOCUMENT NUMBER: 137:263032

TITLE: Preparation of imidazoles as selective agonists at .alpha.2B or .alpha.2B/.alpha.2C adrenergic receptors INVENTOR(S):

Chow, Ken; Gil, Daniel W.; Burke, James A.; Harcourt, Dale A.; Garst, Michael E.; Wheeler, Larry A.; Munk,

Stephen A.; Gomez, Dario G.

Allergan, Inc., USA PATENT ASSIGNEE(S):

PCT Int. Appl., 141 pp. CODEN: PIXXD2 SOURCE:

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

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WO 2002-US8222 W 20020313 OTHER SOURCE(S): MARPAT 137:263032

$$(\mathbb{R}^{1})_{\mathbb{R}}$$

$$(\mathbb{R}^{2})_{\mathbb{R}}$$

$$(\mathbb{R}^{3})_{\mathbb{R}}$$

PRI

Compds. (shown as I), which are selective agonists at .alpha.2B or .alpha.2B/.alpha.2C adrenergic receptors and useful for the treatment of conditions including pain, particularly chronic pain, glaucoma or elevated intraocular pressure with reduced cardiovascular or sedative side effects, are claimed. Also included are methods of making and using such compds.

ANSWER 4 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) 1H-Imidazole, 4-[(1,2,3,4-tetrahydro-4,4-dimethyl-2-naphthalenyl)methyl]-226571-36-4P, 1H-Imidazole, 4-[(1,2,3,4-tetrahydro-7-methyl-2naphthalenyl)methyl]-, monohydrochloride 226571-37-5P, 1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-7-methyl-RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(prepn. of imidazoles as selective agonists at .alpha.2b or

.alpha.2b/.alpha.2c adrenergic receptors)

157058-44-1 CAPLUS

1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)- (9CI) (CA

157058-52-1 CAPLUS

 $\label{localization} $$1$H-Imidazole, $4-[(1,2,3,4-tetrahydro-2-naphthalenyl) methyl]- (9CI) $$ (CA)$ and $$(2,3,4-tetrahydro-2-naphthalenyl) methyl]- (9CI) $$ (CA)$ and $$(2,3,4-tetrahydro-2-naphthalenyl) methyl]- (9CI) $$ (CA)$ (CA) $$ (CA) $$ (CA)$ (CA) $$ (CA)$ (CA) $$ (CA)$ (CA) $$ (CA)$ (CA) $$ (CA) $$ (CA)$ (CA) $$ (CA)$ (CA) $$ (CA)$ (CA) $$ (CA)$ (CA) $$ (CA) $$ (CA)$ (CA) $$ (CA)$ (CA) $$ (CA)$ (CA) $$ (CA)$ (CA) $$ (CA) $$ (CA)$ (CA$ CN INDEX NAME)

157058-55-4 CAPLUS

1H-Imidazole, 4-[(1,2,3,4-tetrahydro-7-methoxy-2-naphthalenyl)methyl]-(9CI) (CA INDEX NAME)

1H-Imidazole, 4-[(1,2,3,4-tetrahydro-7-methoxy-2-naphthalenyl)methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

Page 13 01/13/2004

ANSWER 4 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

226571-02-4 CAPLUS RN

1(2H) -Naphthalenone, 3,4,5,6,7,8-hexahydro-2-(1H-imidazol-4-ylmethyl)-(9CI) (CA INDEX NAME)

226571-05-7 CAPLUS

1H-Imidazole, 4-[(1,2,3,4,5,6,7,8-octahydro-2-naphthalenyl)methyl]- (9CI) . (CA INDEX NAME)

$$CH_2$$

226571-13-7 CAPLUS

1H-Imidazole, 4-[[(2S)-1,2,3,4-tetrahydro-2-naphthalenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

226571-14-8 CAPLUS

1H-Imidazole, 4-[[(2R)-1,2,3,4-tetrahydro-2-naphthalenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

226571-25-1 CAPLUS

1H-Imidazole, 4-[(1,2,3,4-tetrahydro-4-methyl-2-naphthalenyl)methyl]~
(9CI) (CA INDEX NAME)

ANSWER 4 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

226571-57-9P, 1-Naphthalenol, 1,2,3,4-tetrahydro-2-(1H-imidazol-4ylmethyl) -7-methoxy-RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT

(Reactant or reagent) (prepn. of imidazoles as selective agonists at .alpha.2b or

.alpha.2b/.alpha.2c adrenergic receptors) 226571-57-9 CAPLUS

1-Naphthalenol, 1,2,3,4-tetrahydro-2-(1H-imidazol-4-ylmethyl)-7-methoxy-(9CI) (CA INDEX NAME)

ANSWER 4 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

226571-26-2 CAPLUS

1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-4-methyl-(9CI) (CA INDEX NAME)

226571-35-3 CAPLUS

IH-Imidazole, 4-[(1,2,3,4-tetrahydro-4,4-dimethyl-2-naphthalenyl)methyl]-(9CI) (CA INDEX NAME)

226571-36-4 CAPLUS

CN 1H-Imidazole, 4-[(1,2,3,4-tetrahydro-7-methyl-2-naphthalenyl)methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\mathsf{Me} = \mathsf{CH}_2 - \mathsf{CH}_2 - \mathsf{M}_N$$

HC1

226571-37-5 CAPLUS

1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-7-methyl-(9CI) (CA INDEX NAME)

L6 ANSWER 5 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: DOCUMENT NUMBER:

TITLE:

2002:576071 CAPLUS

137:262610 Highly Enantioselective Reformatskii Reaction of

Ketones: Chelation-Assisted Enantioface Discrimination Ojida, Akio; Yamano, Toru; Taya, Naohiro; Tasaka,

AUTHOR(S):

Akihiro

CORPORATE SOURCE: Medicinal Chemistry Research Laboratories, Takeda Chemical Industries, Ltd., Osaka, 532-8686, Japan

SOURCE: Organic Letters (2002), 4(18), 3051-3054 CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

Highly enantioselective Reformatskii reaction of ketones was accomplished using cinchona alkaloids as chiral ligands. Chelation with the sp2-nitrogen adjacent to the reactive carbonyl center contributed to the

enantioface discrimination for the high enanticselectivities.

463304-63-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(chelation-assisted enantioface discrimination in asym. Reformatskii reactions)

463304-63-4 CAPLUS

2-0xazolidinone, 3-[(3S)-3-hydroxy-3-(1H-imidazol-4-yl)-3-(2-naphthalenyl)-1-oxopropyl]-4-phenyl-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

463304-62-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(chelation-assisted enantioface discrimination in asym. Reformatskii

reactions) 463304-62-3 CAPLUS

1,3-Propanediol, 1-(1H-imidazol-4-yl)-1-(2-naphthalenyl)-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS

Page 14 01/13/2004

L6 ANSWER 5 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 6 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) imidazol-4-yl)-2-methylpropyl]-1,2-dihydro-3H-benzo[e]isoindol-3-one inhibited the biosynthesis of testosterone in rats. Formulations are

430472-30-3P 430472-32-5P 430472-34-7P 430472-36-9P 430472-38-1P 430472-39-2P 430472-40-5P 430472-41-6P 430472-42-7P 430472-43-8P 430472-44-9P 430472-45-0P 430472-46-1P 430472-47-2P 430472-48-3P 430472-49-4P 430472-51-8P 430472-53-0P

RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of imidazole derivs. for treatment of prostate and breast

430472-30-3 CAPLUS

3H-Benz[e]isoindol-3-one, 1,2-dihydro-7-[1-hydroxy-1-(1H-imidazol-4-ył)-2-methylpropyl]- (9CI) (CA INDEX NAME)

430472-32-5 CAPLUS

3H-Benz[e]isoindol-3-one, 1,2-dihydro-7-[1-hydroxy-1-(1H-imidazol-4-yl)-2methylpropyl]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & i - Pr & H \\ \hline & N & OH & N \end{array}$$

430472-34-7 CAPLUS

3H-Benz[e]isoindol-3-one, 2-ethyl-1,2-dihydro-7-[1-hydroxy-1-(1H-imidazol-

4-y1)-2-methylpropy1]- (9CI) (CA INDEX NAME)

430472-36-9 CAPLUS

L6 ANSWER 6 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:391704 CAPLUS

DOCUMENT NUMBER: 136:401756

Preparation of imidazole derivatives for treatment of

prostate and breast cancer INVENTOR(S): Tasaka, Akihiro: Matsunaga, Nobuyuki: Ojida, Akio:

Kusaka, Masami PATENT ASSIGNEE(S):

Takeda Chemical Industries, Ltd., Japan SOURCE:

PCT Int. Appl., 81 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

> PATENT NO. KIND DATE APPLICATION NO. DATE WO 2001-JP10079 20011119 WO 2002040470 A1 20020523 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, S1, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG 014320 A5 20020527 AU 2002-14320 20011119 241377 A2 20020828 JP 2001-353524 20011119 777 A1 20030917 EP 2001-982839 20011119 AU 2002014320 JP 2002241377 EP 1344777 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
PRIORITY APPLN. INFO::

JP 2000-382056 A 20001215

WO 2001-JP10079 W 20011119

OTHER SOURCE(S): MARPAT 136:401756

The title compds., e.g. I [R is hydrogen or a protecting group: R1 is lower alkyl or cycloalkyl; and ring A is an optionally substituted 5- or 6-membered ring having an amide linkage], are prepd. I are steroid C17-20 lyase inhibitors and are useful in the treatment of prostate and breast cancer. The process for prepg. I is disclosed. 7-[1-Hydroxy-1-(1H-

ANSWER 6 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) 3H-Benz[e]isoindol-3-one, 1,2-dihydro-7-[1-hydroxy-1-(1H-imidazol-4-yl)-2methylpropyl] -2-propyl- (9CI) (CA INDEX NAME)

430472-38-1 CAPLUS

3H-Benz(e]isoindol-3-one, 1,2-dihydro-7-[1-hydroxy-1-(1H-imidazol-4-yl)-2methylpropyl] -2-(1-methylethyl) - (9CI) (CA INDEX NAME)

430472-39-2 CAPLUS

3H-Benz[e]isoindol-3-one, 2-cyclopropyl-1,2-dihydro-7-[1-hydroxy-1-(1Himidazol-4-yl)-2-methylpropyl]- (9CI) (CA INDEX NAME)

430472-40-5 CAPLUS

JH-Benz[e]isoindol-3-one, 1,2-dihydro-7-[1-hydroxy-1-(1H-imidazol-4-yl)-2methylpropyl) -2-(2,2,2-trifluoroethyl) - (9CI) (CA INDEX NAME)

430472-41-6 CAPLUS

Page 15 01/13/2004

L6 ANSWER 6 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN 3H-Benz[e]isoindol-3-one, 2-(dimethylamino)-1,2-dihydro-7-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]- (9CI) (CA INDEX NAME)

RN 430472-42-7 CAPLUS
CN Benzo[f]phthalazin-4(1H)-one, 2,3-dihydro-8-[1-hydroxy-1-(1H-imidazol-4-y1)-2-methylpropy1]- (9CI) (CA INDEX NAME)

RN 430472-43-8 CAPLUS
CN Benzo[f]phthalazin-4(3H)-one, 8-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]- (9CI) (CA INDEX NAME)

RN 430472-44-9 CAPLUS
CN 1H-Benz[f]isoindol-1-one, 2,3-dihydro-6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]- (9CI) (CA INDEX NAME)

L6 ANSWER 6 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 430472-49-4 CAPLUS
CN 3H-Benz[e]isoindol-3-one, 1,2-dihydro-7-[1-hydroxy-1-(1H-imidazol-4-yl)-3-methylbutyl]-2-methyl- (9CI) (CA INDEX NAME)

RN 430472-51-8 CAPLUS
CN 3H-Benz[e]isoindol-3-one, 1,2-dihydro-7-{l-hydroxy-1-(lH-imidazol-4-yl)-2-methylpropyl]-2-methyl-, (-)- (9CI) (CA INDEX NAME)

Rotation (-).

RN 430472-53-0 CAPLUS
CN 3H-Benz[e]isoindol-3-one, 1,2-dihydro-7-{1-hydroxy-1-(1H-imidazol-4-yl)propyl]-2-methyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS

6 ANSWER 6 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 430472-45-0 CAPLUS
CN 1H-Benz[f]isoindol-1-one, 2,3-dihydro-6-[1-hydroxy-1-(1H-imidazol-4-y1)-2-methylpropyl]-2-methyl- (9C1) (CA INDEX NAME)

RN 430472-46-1 CAPLUS
CN Benzo[g]phthalazin-1(2H)-one, 3,4-dihydro-7-(1-hydroxy-1-(1H-imidazol-4-y1)-2-methylpropyl]- (9CI) (CA INDEX NAME)

RN 430472-47-2 CAPLUS
CN Benzo[g]phthalazin-1(2H)-one, 7-{1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]- (9CI) (CA INDEX NAME)

RN 430472-48-3 CAPLUS
CN 3H-Benz[e]isoindol-3-one, 1,2-dihydro-7-[1-hydroxy-1-(1H-imidazol-4-y1)ethy1]-2-methy1- (9CI) (CA INDEX NAME)

L6 ANSWER 6 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L6 ANSWER 7 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:
                                 2002:353314 CAPLUS
                                 136:365878
DOCUMENT NUMBER:
                                 Methods and compositions for treatment of ocular
TITLE:
                                 neovascularization and neural injury
INVENTOR(S):
                                 Burke, James A.; Lin, Ton: Wheeler, Larry A.; De
                                 Vries, Gerald W.
PATENT ASSIGNEE(S):
                                 Allergan Sales, Inc., USA
                                 PCT Int. Appl., 31 pp. CODEN: PIXXD2
SOURCE:
DOCUMENT TYPE:
                                 Patent
LANGUAGE:
                                 English
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                                                         APPLICATION NO. DATE
      PATENT NO.
                             KIND DATE
      WO 2002036162
                                                         WO 2001~US46014 20011101
      WO 2002036162
                              A3
                                    20030821
            W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
                CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ,
                 VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
            RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
                DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG 030567 A5 20020515 AU 2002-30567 20011101 094998 A1 20020718 US 2001-998718 20011101
      AU 2002030567
      US 2002094998
                             A2 20031022
                                                        EP 2001-990804
      EP 1353692
           R: AT, BE, CH, DE, DK, ES, FR, GB, GR, 1T, L1, LU, NL, SE, MC, PT,
      IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
US 2003092183 A1 20030501 US 2002-20541 20020426
RITY APPLN. INFO.: US 2000-244850P P 20001101
PRIORITY APPLN. INFO.:
                                                    WO 2001-US46014 W 20011101
     Methods and compns. for the treatment of ocular neovascularization (CNV)
      and macular degeneration are disclosed. The invention includes combining
      laser treatment with administration of a neuroprotectant. Seven pigmented rabbits were dosed with either 0.5 mL 0.2% brimonidine or saline administered in 1 eye of each rabbit. One hour later, the animals were
      treated with a 10-min i.v. infusion of 0.2 mg/kg verteporfin, then the
      same eye was irradiated 10 min later in the lower fundus with a 689-nm
      diode laser at 50 J/cm2, 600 mW/cm2 and a spot size of 1.5 mm.
      Brimonidine reduced the increase in retinal thickness (subretinal cyst +
     retina) in the lesion produced by PDT.
226571-05-7, AGN 795 423773-40-4, AGN 960
      RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
      (Biological study); USES (Uses)
          (methods and compns. for treatment of ocular neovascularization and
          neural injury)
      226571-05-7 CAPLUS

1H-Imidazole, 4-[(1,2,3,4,5,6,7,8-octahydro-2-naphthalenyl)methyl]- (9CI)
      (CA INDEX NAME)
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DOCUMENT NUMBER: 136:146981 TITLE: Investigations on inhibitors of human 17.alpha.-hydroxylase-17,20-lyase and their interactions with the enzyme. Molecular modelling of 17.alpha.-hydroxylase-17,20-lyase, part II AUTHOR(S): Schappach, A.; Holtje, H.-D. CORPORATE SOURCE: Department of Pharmacy, Institute of Pharmaceutical Chemistry, Heinrich Heine-University, Dusseldorf, Germany Pharmazie (2001), 56(11), 835-842 SOURCE: CODEN: PHARAT; ISSN: 0031-7144 PUBLISHER: Govi-Verlag Pharmazeutischer Verlag DOCUMENT TYPE: Journal English New methods in treatment of hormone-dependent diseases like prostate or breast cancer have become a major subject in medical and pharmaceutical research. Because of the direct correlation of cancer growth and hormone concn., inhibition of hormone biosynthesis presents a promising strategy in cancer therapy. The key enzyme in androgen biosynthesis is the 17.alpha.-hydroxylase-17,20-lyase a cytochrome P 450 system, which specifically converts gestagens to androgens. Because the 3D-structure of the enzyme is still unknown most recently a ligand-based design was used to gain deeper insights into protein structure and function. In this paper we present mol. modeling studies on compds. acting as competitive inhibitors of the human 17.alpha.-hydroxylase-17,20-lyase. The compds. developed by Hartmann et al. belong to two different structural classes and show a wide range of inhibitory potency. The physico-chem. properties of the mols. were investigated and compared by studying structural flexibility and by calcg. mol. interactions fields. The superimposition of all inhibitors in a low energy conformation yielded in the common pharmacophore. In the second part of the paper individual inhibitors were docked into the active site of the enzyme model of CYP17 developed in our group. The dynamic behavior and stability of the protein-inhibitorcomplexes was studied. The protein ligand interactions obsd. in course of the mol. dynamics simulations correspond well with the exptl. data. 157058-47-4 RL: PRP (Properties) (mol. modeling of human 17.alpha.-hydroxylase-17,20-lyase with

1(2H) -Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-7-methoxy-

L6 ANSWER 8 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

steroidal and non-steroidal inhibitors

2001:848687 CAPLUS

ACCESSION NUMBER:

157058-47-4 CAPLUS

(9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT ANSWER 7 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

423773-40-4 CAPLUS

1(2H)-Naphthalenone, 2-[(2,3-dihydro-2-thioxo-1H-imidazol-4-yl)methyl]-3,4dihydro- (9CI) (CA INDEX NAME)

L6 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 2001:319877 CAPLUS DOCUMENT NUMBER: 134:340525

TITLE: Process for producing optically active naphthalene

derivative and optical resolver therefor INVENTOR (S): Aoki, Isao; Adachi, Mari: Kawada, Mitsuru; Yamano,

Toru; Taya, Nachiro

PATENT ASSIGNEE(\$): Takeda Chemical Industries, Ltd., Japan SOURCE:

PCT Int. Appl., 103 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PAT	PENT	NO.			ND	DATE					CATI			DATE			
WO	2001	0307	63											2000	1019		
	W:	ΑE,	AG,	AL,	AM,	ΑU,	AZ,	BA,	BB,	₿G,	BR,	BY,	ΒZ,	CA,	CN,	CR,	CU,
		CZ,	DM,	DZ,	EE,	GD,	GE,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KG,	KR,	KZ,
		LC,	LK,	LR,	LT,	LV,	MA,	MD,	MG,	MK,	MN,	MX,	NO,	NZ,	PL,	RO,	RU,
		\$G,	51,	SK,	TJ,	TM,	TR,	TT,	UA,	US,	UZ,	VN,	YU,	ZA,	AM,	AZ,	BY,
		KG,	KZ,	MD,	RU,	ТJ,	TM										
	R₩:	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	Т2,	UG,	ZW,	AT,	BE,	CH,	CY,
		DE,	DK,	E5,	FI,	FR,	GB,	GR,	IE,	ΙT,	LU,	MC,	NL,	-PT,	SE,	BF,	BJ,
		CF,	CG,	CI,	CM,	GA,	GN,	G₩,	ML,	MR,	NE,	SN,	TD,	TG			
ΑU	2000	07949	99	A!	5	2001	0508		A	U 201	20-79	9499		2000	1019		
ΕP	1227	085		A.	1	2002	0731		E	P 20	00-96	5990	2	2000	1019		
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY.	AL						-	
JР	2001	18778	95	A.	2	2001	0710		J	P 200	00-32	20499	9	2000	1020		
RT I	APP.	LN.	INFO	. :				,	JP 19	999-	3015	70	A	1999	1022		
														1999			
								1	WO 20	000-	JP728	12	W	2000	1019		
8 50	URCE	(5):			MAR	PAT	134:3					_					

OTH

PRI

AT 134:34U525

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

A process for producing an optically active isomer of a compd. represented by formula (1) which comprises: reacting a mixt. of naphthalene derivs. represented by formula I (wherein R represents a nitrogenous heterocyclic group; R1 represents hydrogen, a hydrocarbon group, or a mononuclear arom. heterocyclic group; R2 represents hydrogen or lower alkyl; symbol indicates the position of an asym. carbon atom; and R3 to R8 each represents hydrogen, a hydrocarbon group, hydroxy, etc., provided that R7 may be bonded to R6 or R8 to form a ring contg. an oxygen atom) with an optically active isomer of a 2-hydroxy-4-phenyl-1,3,2-dioxaphosphorinan-2one or arom. ring-fused 2-hydroxy-1,3,2-dioxaphosphepan-2-one compd. represented by formula (II) or (III), resp. (wherein ring A represents a benzene ring: R10 and R11 each represents hydrogen, a hydrocarbon group, etc. or R10 and R11 in combination represent alkylene; symbol indicates the position of an asym. carbon atom; and rings B and C each represents an arom. ring) to yield salts; sepg. the salts; and then isolating the target isomer. The optically active isomer produced has a steroid C17,20 lyase inhibitory activity and is useful as a preventive/remedy for tumors such as prostatism and mammary cancer. Also provided is a novel optical resolver II or III. Thus, 1.0 g (RS)-1-(6,7-dimethoxynaphthalen-2-yl)-1-

Page 17 01/13/2004

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) (lH-imidazol-4-yl)-2-methyl-1-propanol (IV) (prepn. given) and 822 mg (-)-8-hydroxy-7,9-dioxa-6-phenyl-8-phopehaspiro[4.5]decan-8-one (V) were dissolved in 21 mL ethanol with heating, stirred at room temp. for 6 h, and filtered to give 670 mg (-)-IV.V salt (99% de) in 74% yield which (665 mg) was added to 150 mg 25% aq. NH3, 30 mL H2O, and 20 mL AcOEt, and stirred at room temp. for 30 min. The org. layer was sepd. and concd. in vacuo to give 368 mg (-)-IV (99% de) in 74% yield. 336102-55-7P 336102-62-6P

RL: PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(process for producing optically active anticancer naphthalene deriv. and hydroxyphenyldioxaphosphorinanone resolving agents) 336102-55-7 CAPLUS

IH-Imidazole-4-methanol, .alpha.-(6,7-dimethoxy-2-naphthalenyl)-.alpha.-(1methylethyl) -, (.alpha.5) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

336102-62-6 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(6-methoxy-2-naphthalenyl)-.alpha.-(1methylethyl) -, (-) - (9CI) (CA INDEX NAME)

Rotation (-).

336102-65-9 336102-70-6 336102-73-9 ΙT

RL: RCT (Reactant); RACT (Reactant or reagent) (process for producing optically active anticancer naphthalene deriv. and hydroxyphenyldioxaphosphorinanone resolving agents) 336102-65-9 CAPLUS

2-Naphthalenecarboxylic acid, 6-[1-hydroxy-1-(1H-imidazol-4-yl)-3methylbutyl]-, methyl ester (9CI) (CA INDEX NAME)

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

247173-20-2 CAPLUS

CN 1H-Imidazole-4-methanol, .alpha.-(6-methoxy-2-naphthalenyl)-.alpha.-propyl-(9CI) (CA INDEX NAME)

247173-40-6 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(6-ethoxy-2-naphthalenyl)-.alpha.-(1methylethyl) - (9CI) (CA INDEX NAME)

RN 247173-41-7 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(6,7-dimethoxy-2-naphthalenyl)-.alpha.-(1-CN methylethyl) - (9CI) (CA INDEX NAME)

247173-54-2 CAPLUS CN Acetamide, N-[6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2-

naphthalenyl] - (9CI) (CA INDEX NAME)

247173-72-4 CAPLUS

CN Methanone, 1H-imidazol-4-yl(6-methoxy-2-naphthalenyl)- (9CI) (CA INDEX NAME)

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

336102-70-6 CAPLUS

2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-yl)-3-methylbutyl]-N-methyl- (9CI) (CA INDEX NAME)

336102-73-9 CAPLUS

2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazo1-4-yl)propyl]-Nmethyl- (9CI) (CA INDEX NAME)

247173-05-3P 247173-20-2P 247173-40-6P

247173-41-7P 247173-54-2P 247173-72-4P

247174-12-5P 336102-57-9P 336102-59-1P 336102-61-5P 336102-63-7P 336102-64-8P

336102-66-0P 336102-67-1P 336102-69-3P

336102-71-7P 336102-72-8P 336102-74-0P 336102-75-1P 336102-76-2P 337534-07-3P

337534-08-4P 337534-10-8P 337534-11-9P

RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)

(process for producing optically active anticancer naphthalene deriv.

and hydroxyphenyldioxaphosphorinanone resolving agents)

247173-05-3 CAPLUS
1H-Imidazole-4-methanol, .alpha.-(6-methoxy-2-naphthalenyl)-.alpha.-(1-methylethyl)- (9C1) (CA INDEX NAME)

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

247174-12-5 CAPLUS

Methanone, (6,7-dimethoxy-2-naphthalenyl)-1H-imidazel-4-yl- (9CI) (CA INDEX NAME) CN

336102-57-9 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(6,7-dimethoxy-2-naphthalenyl)-.alpha.-(1-methylethyl)-, (.alpha.S)-, compd. with (-)-8-hydroxy-6-phenyl-7,9-dioxa-8-phosphaspiro[4.5]decame 8-oxide (1:1) (9CI) (CA INDEX NAME)

CM

CRN 336102-56-8 CMF C13 H17 O4 P

Rotation (-).

CRN 336102-55-7 CMF C19 H22 N2 O3

Absolute stereochemistry. Rotation (-).

336102-59-1 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(6-ethoxy-2-naphthalenyl)-.alpha.-(1methylethyl)-, (-)-, compd. with (45)-4-(2,4-dichlorophenyl)-2-hydroxy-5,5-

Page 18 01/13/2004

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) dimethyl-1,3,2-dioxaphosphorinane 2-oxide (1:1) (9CI) (CA INDEX NAME)

CRN 336102-58-0 CMF C19 H22 N2 O2

Rotation (-).

CM

CRN 98674-91-0

CMF C11 H13 C12 O4 P

Absolute stereochemistry. Rotation (-).

336102-61-5 CAPLUS

Acetamide, N-[6-[1-hydroxy-1-(1H-imidazol-4-y1)-2-methylpropy1]-2-naphthalenyl]-, (+)-, compd. with (+)-2-hydroxy-4-(2-methoxyphenyl)-5,5dimethy1-1,3,2-dioxaphosphorinane 2-oxide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 336102-60-4

CMF C19 H21 N3 O2

Rotation (+).

L6 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) Rotation (-).

1H-Imidazole-4-methanol, .alpha.-(6-methoxy-2-naphthalenyl)-.alpha.-(1methylethyl)-, (-)-, compd. with (4S)-2-hydroxy-4-(2-methoxyphenyl)-5,5dimethyl-1,3,2-dioxaphosphorinane 2-oxide (1:1) (9CI) (CA INDEX NAME)

CRN 336102-62-6 CMF C18 H20 N2 O2

Rotation (-).

CM 2

CRN 98674-83-0 CMF C12 H17 O5 P

Absolute stereochemistry. Rotation (-).

336102-66-0 CAPLUS

2-Naphthalenecarboxylic acid, 6-[1-hydroxy-1-(1H-imidazol-4-yl)-3-methylbutyl]-, methyl ester, compd. with (4R)-4-(2-chlorophenyl)-2-hydroxy-5,5-dimethyl-1,3,2-dioxaphosphorinane 2-oxide (1:1) (9CI) (CA INDEX NAME)

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

CM

CRN 98674-82-9 CMF C12 H17 O5 P

Absolute stereochemistry. Rotation (+).

336102-63-7 CAPLUS

1H-Imidazole-4-methanol, .alpha.~(6-methoxy-2-naphthalenyl)-.alpha.~(1methylethyl)-, (-)-, compd. with (-)-4-(4-chlorophenyl)-2-hydroxy-5,5-dimethyl-1,3,2-dioxaphosphorinane 2-oxide (1:1) (9C1) (CA INDEX NAME)

CRN 336102-62-6 CMF C18 H20 N2 O2

Rotation (-).

CM

CRN 98674-89-6 CMF C11 H14 C1 O4 P

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) CRN 336102-65-9 CMF C20 H22 N2 O3

CM 2

CRN 98674-87-4 CMF C11 H14 C1 O4 P

Absolute stereochemistry. Rotation (+).

336102-67-1 CAPLUS

2-Naphthalenecarboxylic acid, 6-[1-hydroxy-1-(1H-imidazol-4-yl)-3methylbutyl]-, methyl ester, compd. with (+)-4-(2,4-dichlorophenyl)-2-hydroxy-5,5-dimethyl-1,3,2-dioxaphosphorinane 2-oxide (1:1) (9CI) (CA

CM 1

CRN 336102-65-9 CMF C20 H22 N2 03

CM

CRN 98674-90-9 CMF C11 H13 C12 O4 P

Absolute stereochemistry. Rotation (+).

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L6 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS OR STN (Continued)

336102-69-3 CAPLUS

2-Naphthalenecarboxylic acid, 6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-, methyl ester, compd. with (4S)-4-(2-chlorophenyl)-2-hydroxy-5,5-dimethyl-1,3,2-dioxaphosphorinane 2-oxide (1:1) (9CI) (CA) INDEX NAME)

CM 1

CRN 336102-68-2 CMF C19 H20 N2 O3

CM 2

CRN 98674-86-3 CMF C11 H14 C1 04 P

Absolute stereochemistry. Rotation (-).

336102-71-7 CAPLUS

2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-yl)-3-methylbutyl]-N-methyl-, compd. with (4R)-4-(2-chlorophenyl)-2-hydroxy-5,5-dimethyl-1,3,2-dioxaphosphorinane 2-oxide (1:1) (9CI) (CA INDEX NAME)

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) CM 2

CRN 98674-91-0 CMF C11 H13 C12 O4 P

Absolute stereochemistry. Rotation (-).

336102-74-0 CAPLUS

2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-yl)propyl]-Nmethyl-, compd. with (+)-4-(2,4-dichlorophenyl)-2-hydroxy-5,5-dimethyl-1,3,2-dioxaphosphorinane 2-oxide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 336102-73-9

CMF C18 H19 N3 02

CM 2

CRN 98674-90-9 CMF C11 H13 C12 04 P

Absolute stereochemistry. Rotation (+).

336102-75-1 CAPLUS

2-Naphthalenecarboxamide, 6-[1-hydroxy-1-{1H-imidazol-4-yl)propyl}-Nmethyl-, compd. with (4R)-4-(2-chlorophenyl)-2-hydroxy-5,5-dimethyl-1,3,2L6 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

CM 1

CRN 336102-70-6 CMF C20 H23 N3 O2

CM 2

CRN 98674-87-4 CMF C11 H14 C1 04 P

Absolute stereochemistry. Rotation (+).

336102-72-8 CAPLUS

2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-y1)-3-methylbuty1]-N-methyl-, compd. with (-)-4-(2,4-dichlorophenyl)-2-hydroxy-5,5-dimethyl-1,3,2-dioxaphosphorinane 2-oxide (1:1) (9CI) (CA INDEX NAME)

CRN 336102-70-6 CMF C20 H23 N3 O2

L6 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN dioxaphosphorinane 2-oxide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 336102-73-9 CMF C18 H19 N3 O2

CM

CRN 98674-87-4 CMF C11 H14 C1 O4 P

Absolute stereochemistry. Rotation (+).

336102-76-2 CAPLUS
2-Naphthalenecarboxamide, 6-{1-hydroxy-1-(1H-imidazol-4-yl)propyl}-N-methyl-, compd. with (+)-2-hydroxy-4-(2-methoxyphenyl)-5,5-dimethyl-1,3,2-dioxaphosphorinane 2-oxide (1:1) (9CI) (CA INDEX NAME)

CM - 1

CRN 336102-73-9 CMF C18 H19 N3 O2

CRN 98674+82-9

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ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) CMF C12 H17 O5 P

Absolute stereochemistry. Rotation (+).

337534-07-3 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(6,7-dimethoxy-2-naphthalenyl)-.alpha.-(1-methylethyl)-, (-)-, compd. with (11bR)-4-hydroxydinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin 4-oxide (1:1) (9CI) (CA INDEX NAME)

CRN 336102-55-7 CMF C19 H22 N2 O3

Absolute stereochemistry. Rotation (-).

CM

CRN 39648-67-4 CMF C20 H13 O4 P

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

CRN 98674-86-3

CMF C11 H14 C1 O4 P Absolute stereochemistry. Rotation (-).

337534-11-9 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(6-methoxy-2-naphthalenyl)-.alpha.-(1methylethyl)-, (-)-, compd. with (4S)-4-(2-chlorophenyl)-2-hydroxy-5,5dimethyl-1,3,2-dioxaphosphorinane 2-oxide (1:1) (9CI) (CA INDEX NAME)

CM 1

Rotation (-).

CRN 336102-62-6

CMF C18 H20 N2 O2

CTM 2

CRN 98674-86-3

CMF C11 H14 C1 04 P

Absolute stereochemistry. Rotation (-).

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

337534-09-4 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(6,7-dimethoxy-2-naphthalenyl)-.alpha.-(1-methylethyl)-, (-)-, compd. with (4R)-2-hydroxy-5,5-dimethyl-4-phenyl-1,3,2-dioxaphosphorinane 2-oxide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 336102-55-7 CMF C19 H22 N2 03

Absolute stereochemistry. Rotation (-).

CM

CRN 98674-80-7

CMF C11 H15 04 P

Absolute stereochemistry. Rotation (-).

337534-10-8 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(6-methoxy-2-naphthalenyl)-.alpha.-propyl-, (-)-, compd. with (4S)-4-(2-chlorophenyl)-2-hydroxy-5,5-dimethyl-1,3,2-dioxaphosphorinane 2-oxide (1:1) (9CI) (CA INDEX NAME)

CRN 337534-09-5

CMF C18 H20 N2 O2

Rotation (-).

ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

336103-01-6P 336103-02-7P 336103-04-9P

336103-06-1P 337534-12-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (process for producing optically active anticancer naphthalene deriv.

and hydroxyphenyldioxaphosphorinanone resolving agents) 336103-01-6 CAPLUS

Cyclohexanecarboxylic acid, 2-(aminocarbonyl)-, (15,2R)-, compd. with .alpha.-(6,7-dimethoxy-2-naphthalenyl)-.alpha.-(1-methylethyl)-lH-imidazole-4-methanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 336103-00-5

CMF C8 H13 N O3 Absolute stereochemistry.

CRN 247173-41-7 CMF C19 H22 N2 O3

336103-02-7 CAPLUS

Benzeneacetic acid, .alpha.-hydroxy-, (.alpha.S)-, compd. with .alpha.-(6,7-dimethoxy-2-naphthalenyl)-.alpha.-(1-methylethyl)-1Himidazole-4-methanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 247173-41-7

CMF C19 H22 N2 O3

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L6 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

CM

CRN 17199-29-0

CMF C8 H8 03

Absolute stereochemistry. Rotation (+).

Ph

HO₂C

336103-04-9 CAPLUS

2-Naphthalenecarboxamide, 6-[(15)-1-hydroxy-1-(1H-imidazol-4-y1)propyl}-N-methyl-, compd. with (4R)-4-(2-chlorophenyl)-2-hydroxy-5,5-dimethyl-1,3,2-dioxaphosphorinane 2-oxide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 336103-03-8 CMF C18 H19 N3 O2

Absolute stereochemistry. Rotation (-).

CRN 98674-87-4

CMF C11 H14 C1 O4 P

Absolute stereochemistry. Rotation (+).

L6 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) naphthalenyl) -. alpha. - (1-methylethyl) -1H-imidazole-4-methanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 247173-41-7

CMF C19 H22 N2 O3

CM 2

CRN 50573-41-6 CMF C8 H11 N 03 S

Absolute stereochemistry. Rotation (-).

REFERENCE COUNT:

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT L6 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

336103-06-1 CAPLUS

2-Naphthalenecarboxamide, 6-[(1S)-1-hydroxy-1-(1H-imidazo1-4-yl)-3-methylbutyl]-N-methyl-, compd. with (4R)-4-(2-chlorophenyl)-2-hydroxy-5,5-dimethyl-1,3,2-dioxaphosphorinane 2-oxide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 336103-05-0 CMF C20 H23 N3 O2

Absolute stereochemistry.

CM 2

CRN 98674-87-4

CMF C11 H14 Cl 04 P

Absolute stereochemistry. Rotation (+).

337534-12-0 CAPLUS

Sulfamic acid, [(1S)-1-phenylethyl]-, compd. with .alpha.-(6,7-dimethoxy-2-

L6 ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 2001:319876 CAPLUS

DOCUMENT NUMBER: 134:340505

Preparation of imidazol-4-ylmethanols as steroid TITLE:

C17-20 lyase inhibitors Tasaka, Akihiro: Ojida, Akio: Kaku, Tomohiro: Kusaka,

Masami; Yamaoka, Masuo PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 166 pp. CODEN: PIXXD2

Patent

DOCUMENT TYPE: LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

INVENTOR(S):

PATENT NO.	KIN	D DATE		APPLICATION NO. DATE									
WO 2001030	762 A1	20010	503				20001019)					
W: AE	, AG, AL,	AM, AU,	AZ, BA,	вв, в	G, BR,	BY, BZ,	CA, CN,	CR, CU,					
CZ	, DM, DZ, 1	EE, GD,	GE, HR,	HU, I	D, IL,	IN, IS,	JP, KG,	KR, KZ,					
LC	, LK, LR,	LT, LV,	MA, MD,	MG, M	K, MN,	MX, MZ,	NO, NZ,	PL, RO,					
RU	, SG, SI, S	SK, TJ,	TM, TR,	TT, U	A, US,	UZ, VN,	YU, ZA,	AM, AZ,					
FY	', KG, KZ, !	ID, RU,	TJ, TM										
RW: GH	i, GM, KE, I	LS, MW,	MZ, SD,	SL, S	Z, TZ,	UG, ZW,	AT, BE,	CH, CY,					
DE	, DK, E\$, 1	FI, FR,	GB, GR,	IE, I	T, LU,	MC, NL,	PT, SE,	BF, BJ,					
CF	CG, CI, C	M, GA,	GN, GW,	ML, M	R, NE,	SN, TD,	TG						
AU 2000079		20010					20001019						
EP 1222174	A1	20020	717	EP	2000-96	69903	20001019)					
R: AT	, RE, CH, I	DE, DK,	ES, FR,	GB, G	R, IT,	LI, LU,	NL, SE,	MC, PT,					
IE	, SI, LT, 1	LV, FI,	RO, MK,	CY, A	L								
JP 2002080	458 A2	20020	319	JP .	2000-32	27022	20001020)					
U\$ 6649643	B1	20031	118	US .	2002-11	10599	20020412	<u>:</u>					
RIORITY APPLN.	INFO.:			JP 199	9-30155	66 A	19991022	!					
			•	JP 200	0-18972	28 A	20000620	1					
			Ţ	VO 200	0-JP728	3 W	20001019	1					
THER SOURCE(S)	: 1	MARPAT 1	34:34056)5									

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ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

Title compds. (I) {wherein R = H or a protecting group; R1 = (cyclo)alkyl; R3 and R5 = H, acyl, halo, or (un) substituted alkyl, hydroxyl, thio, or amino; R4 = (un)substituted aryl, heterocyclic, or carbamoyl; or R3 and R4 form a 5- or 6-membered O-contg. ring; or R4 and R5 form a 5- or 6-membered O-contg. ring; R6 = (halo)alky1; n=0-3; or salt thereof], which have an inhibitory activity on steroid C17-20 lyase, were prepd. For example, Me 6-(1-hydroxy-2-methyl-1-(1-trityl-1H-imidazol-4-yl)propyl)-2-naphthoate (prepn. given) was deesterified using NaOH and MeOH in THF, converted to the amide using MeNH2, and deprotected using pyridinium chloride to give the imidazolyl naphthalenemethanol II. II inhibited steroid C17-20 lyase with IC50 of 6.1 nM and showed inhibitory activity on testosterone biosynthesis (testosterone concn. of groups of rats receiving test compds. to control groups) of 4.5%. I are useful for the prevention and treatment of breast cancer or prostate cancer (no data).

and treatment of breast cancer of prostate cancer (no data).

247173-41-7P, 1-(6,7-Dimethoxy-2-naphthyl)-1-(1H-imidazol-4-yl)-2methyl-1-propanol 247173-54-2P, N-[6-[1-Hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]naphthalen-2-yl]acetamide
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of imidazolyl naphthalenemethanol steroid C17-20 lyase inhibitors for treatment of breast and prostate cancer)

247173-41-7 CAPLUS
1H-Imidazole-4-methanol, .alpha.-(6,7-dimethoxy-2-naphthalenyl)-.alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME)

247173-54-2 CAPLUS

CN naphthalenyl] - (9CI) (CA INDEX NAME)

336103-03-8P, (S)-(-)-6-[1-Hydroxy-1-(1H-imidazol-4-yl)propyl]-N-methyl-2-naphthamide **337520-97-5P**, 6-[1-Hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2-naphthonitrile **337521-57-0P**, ΙT 6-[1-Hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2-methoxy-N-methyl-1naphthamide 337521-60-5P, 2-Hydroxy-6-[1-hydroxy-1-(1H-imidazol-4-y1)-2-methylpropy1]-N-methyl-1-naphthamide 337521-62-7P, 6-{1-Hydroxy-1-(1H-imidazol-4-y1)-2-methylpropyl}-N-methyl-1-naphthamide 337521-63-8P 337521-94-5P, (1H-Imidazol-4-y1) (naphtho[2,1-b] furan-7-y1) ketone 337521-99-0P, (1H-Imidazol-4-yl)[naphtho[2,3-d][1,3]dioxol-6-yl]ketone

ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) 1-Naphthalenecarboxamide, 2-hydroxy-6-[1-hydroxy-1-(1H-imidazol-4-yl)-2methylpropyl]-N-methyl- (9CI) (CA INDEX NAME)

337521-62-7 CAPLUS

1-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-y1)-2methylpropyl]-N-methyl- (9CI) (CA INDEX NAME)

C-NHMe

337521-63-8 CAPLUS

CN Methanesulfonic acid, trifluoro-, 6-[1-hydroxy-1-(1H-imidazol-4-yl)-2methylpropyl]-1-[(methylamino)carbonyl]-2-naphthalenyl ester (9CI) (CA

337521-94-5 CAPLUS

Methanone, 1H-imidazol-4-ylnaphtho[2,1-b]furan-7-yl- (9CI) (CA INDEX

ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN 337522-08-4P, (2,3-Dihydro-1H-benzo[f]chromen-8-yl) (1H-imidazol-4yl) ketone 337522-19-7P, (1,2-Dihydronaphtho[2,1-b] furan-7-yl) (1Himidazol-4-yl)ketone 337522-26-6P, (2,3-Dihydronaphtho[2,3b]furan-6-yl) (1H-imidazol-4-yl)methanol 337522-27-7P, $\begin{array}{ll} (2,3-\text{Bihydronaphtho}\{2,3-b\}\,\text{furan-6-yl})\,\,(1\text{H-imidazol-4-yl})\,\text{ketone}\\ \textbf{337522-28-8P},\,\,1-\{2,3-\text{Bihydronaphthe}\{2,3-b\}\,\text{furan-6-yl})-1-(1\text{H-imidazol-4-yl})-2-\text{methyl-1-propanol}\,\,\textbf{337534-08-4P} \end{array}$ RL: RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; prepn. of imidazolyl naphthalenemethanol steroid C17-20 lyase inhibitors for treatment of breast and prostate cancer) 336103-03-8 CAPLUS 2-Naphthalenecarboxamide, 6-[(1S)-1-hydroxy-1-(1H-imidazol-4-yl)propyl]-Nmethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

337520-97-5 CAPLUS

2-Naphthalenecarbonitrile, 6-[1-hydroxy-1-(1H-imidazol-4-yl)-2methylpropyl] - (9CI) (CA INDEX NAME)

337521-57-0 CAPLUS

1-Naphthalenecarboxamide, 6-{1-hydroxy-1-(1H-imidazol-4-y1)-2methylpropy1]-2-methoxy-N-methyl- (9CI) (CA INDEX NAME)

337521-60-5 CAPLUS

ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

337521-99-0 CAPLUS

Methanone, 1H-imidazol-4-ylnaphtho[2,3-d]-1,3-dioxol-6-yl- (9CI) (CA CN INDEX NAME)

337522-08-4 CAPLUS

CN Methanone, (2,3-dihydro-1H-naphtho[2,1-b]pyran-8-yl)-1H-imidazol-4-yl-(CA INDEX NAME)

337522-19-7 CAPLUS RN

CN Methanone, (1,2-dihydronaphtho[2,1-b]furan-7-yl)-1H-imidazol-4-yl- (9CI) (CA INDEX NAME)

337522-26-6 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(2,3-dihydronaphtho[2,3-b]furan-6-yl)-

(9CI) (CA INDEX NAME)

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L6 ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 337522-27-7 CAPLUS
CN Methanone, (2,3-dihydronaphtho(2,3-b]furan-6-yl)-1H-imidazol-4-yl- (9CI)
(CA INDEX NAME)

RN 337522-28-8 CAPLUS

CN 1H-Imidazole-4-methanol, .alpha.-(2,3-dihydronaphtho[2,3-b]furan-6-yl)-.alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 337534-08-4 CAPLUS

CN lH-Imidazole-4-methanol, .alpha.-(6,7-dimethoxy-2-naphthalenyl)-.alpha.-(1-methylethyl)-, (-)-, compd. with (4R)-2-hydroxy-5,5-dimethyl-4-phenyl-1,3,2-dioxaphosphorinane 2-oxide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 336102-55-7 CMF C19 H22 N2 03

Absolute stereochemistry. Rotation (-).

CM 2

L6 ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued

RN 337522-94-8 CAPLUS

V 2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-y1)-2-methylpropyl]-N,3-dimethyl- (9CI) (CA INDEX NAME)

RN 337523-27-0 CAPLUS

N Glycine, N-[[6-{1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2-naphthalenyl]carbonyl}-, ethyl ester (9CI) (CA INDEX NAME)

RN 337523-39-4 CAPLUS

CN 2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-yl)ethyl]-N-methyl-(9CI) (CA INDEX NAME)

RN 337523-51-0 CAPLUS

2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazel-4-yl)butyl]-N-methyl-(9CI) (CA INDEX NAME)

RN 337523-67-8 CAPLUS

1H-Imidazole-4-methanol, .alpha.-[5-chloro-6-(1H-1,2,3-triazol-4-yl)-2naphthalenyl]-.alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CRN 98674-80-7
CMF C11 H15 O4 P

Absolute stereochemistry. Rotation (-).

337521-96-7P, 1-(1H-Imidazol-4-yl)-1-[naphtho[2,3-d][1,3]dioxol-6-yl]-2-methyl-1-propanol 337522-45-9P, 6-[1-Hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-N-propyl-2-naphthamide 337522-94-8P, 6-[1-Hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-N,3-dimethyl-2-naphthamide 337523-27-0P, Ethyl {{6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2-naphthoyl]amino}acetate 337523-39-4P, 6-[1-Hydroxy-1-(1H-imidazol-4-yl)ethyl]-N-methyl-2-naphthamide 337523-51-0P, 6-[1-Hydroxy-1-(1H-imidazol-4-yl)butyl]-N-methyl-2-naphthamide 337523-67-8P, 1-[5-Chloro-6-(1H-1,2,3-triazol-4-yl)-2-naphthyl]-1-(1H-imidazol-4-yl)-2-methyl-1-propanol RL: BAC (Biological activity or effector, except adverse): BSU (Biological study, unclassified): RCT (Reactant): SPN (Synthetic preparation): THU (Therapeutic use): BIOL (Biological study): PREP (Preparation): RACT (Reactant or reagent): USES (Uses)

(prepn. of imidazolyl naphthalenemethanol steroid C17-20 lyase inhibitors for treatment of breast and prostate cancer) 337521-96-7 CAPLUS

N IH-Imidazole-4-methanol, .alpha.-(1-methylethyl)-.alpha.-naphtho[2,3-d]-1,3-dioxol-6-yl- (9CI) (CA INDEX NAME)

RN 337522-45-9 CAPLUS

CN 2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-N-propyl- (9CI) (CA INDEX NAME)

L6 ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

336102-55-7P, (S)-(-)-1-(6,7-Dimethoxy-2-naphthyl)-1-(1H-imidazol-4-yl)-2-methyl-1-propanol 336102-68-2P, Methyl 6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2-naphthoate 336102-70-6P, 6-[1-Hydroxy-1-(1H-imidazol-4-yl)-3-methylbutyl]-N-methyl-2-naphthamide 336102-73-9P, 6-[1-Hydroxy-1-(1H-imidazol-4-yl)propyl]-N-methyl-2-naphthamide 337521-66-1P, 1-(IH-Imidazol-4-yl)-2-methyl-1-(6-phenyl-2-naphthyl)-1-propanol 337521-68-3P, 1-[6-(2-Furyl)-2-naphthyl]-1-(lH-imidazol-4-yl)-2-methyl-1-propanol 337521-70-7P, 1-(lH-Imidazol-4-yl)-2-methyl-1-[6-(2-thienyl)-2-naphthyl]-1-propanol 337521-74-1P, 1-(1H-Imidazol-4-yl)-2-methyl-1-[6-(1H-1,2,3-triazol-4-yl)-2-naphthyl]-1propanol 337521-77-4P, 1-(1H-Imidazol-4-yl)-2-methyl-1-[6-(1H-1,2,3,4-tetrazol-5-yl)-2-naphthyl]-1-propanol 337521-79-6P, 1-(lH-Imidazol-4-yl)-2-methyl-1-[6-(lH-pyrazol-4-yl)-2-naphthyl]-1-propanol 337521-81-0P, 1-(lH-Imidazol-4-yl)-2-methyl-1-[6-(l,3oxazol-5-yl)-2-naphthyl]-1-propanol 337521-84-3P, 6-[1-Hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-N-methyl-2-naphthamide 337521-86-5P, 6-[1-Hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-Nmethoxy-2-naphthamide 337521-89-8P, 1-(1H-Imidazol-4-yl)-1-(naphtho[2,1-b]furan-7-yl)-2-methyl-1-propanol 337521-95-6P,
1-(1,2-Dihydronaphtho[2,1-b]furan-7-yl)-1-(1H-imidazol-4-yl)-2-methyl-1propanol 337522-00-6P, 1-(2,3-Dihydro-1H-benzo[f]chromen-8-yl)-1(1H-imidazol-4-yl)-2-methyl-1-propanol 337522-09-5P, 1-(2,3-Dihydro-1H-benzo[f]chromen-8-yl)-1-(1H-imidazol-4-yl)ethanol 337522-10-8P, 1-(2,3-Dihydro-lH-benzo[f]chromen-8-yl)-1-(lH-imidazol-4-yl)propanol 337522-12-0P, 1-(1,2-Dihydronaphtho{2,1-imidazol-4-yl)-2-methylpropyl]naphthalen-2-yl]acetamide 337522-40-4P 337522-41-5P, N-Ethyl-6-[1-hydroxy-1-(1Himidazol-4-yl)-2-methylpropyl]-2-naphthamide 337522-49-3P,
6-[1-Hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-N-isopropyl-2naphthamide 337522-53-9P, N-Butyl-6-(1-hydroxy-1-(1H-imidazol-4y1) -2-methylpropy1] -2-naphthamide 337522-57-3P, N-Cyclopropyl-6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl}-2naphthamide 337522-61-9P, N-Cyclobutyl-6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2-naphthamide 337522-64-2P, N-Cyclopropylmethyl-6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2-naphthamide 337522-67-5P, N-Cyclopentyl-6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl)-2-naphthamide 337522-67-5P, N-Cyclopentyl-6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl)-2-methylpropyl-1-(1H-imidazol-4-yl)-2-methylpropyl-2-methylpropyl-1-(1H-imidazol-4-yl)-2-methylpropyl-2-methyl imidazol-4-y1)-2-methylpropyl]-2-naphthamide 337522-69-7P, N-Cyclohexyl-6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2naphthamide 337522-72-2P, N-Cycloheptyl-6-[1-hydroxy-1-(1H imidazol-4-yl)-2-methylpropyl]-2-naphthamide 337522-74-4P, 6-[1-Hydroxy-1-(lH-imidazol-4-yl)-2-methylpropyl]-2-naphthamide 337522-77-7P, 1-Chloro-6-{1-hydroxy-1-(1H-imidazol-4-yl)-2methylpropyl]-2-naphthamide 337522-79-9P, 6-[1-Hydroxy-1-(1H $imidazol-4-yl)-2-methylpropyl]-1-methyl-2-naphthamide \ \textbf{337522-83-5P}$, 1-Chloro-6-[1-hydroxy-1-(lH-imidazol-4-yl)-2-methylpropyl]-N-methyl-2-naphthamide 337522-88-0P, 6-[1-Hydroxy-1-(lH-imidazol-4-yl)-2-

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ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) methylpropyl]-N, 1-dimethyl-2-naphthamide 337522-99-3P, 6-[1-Hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-3-methyl-2-naphthamide 337523-03-2P, 6-[1-Hydroxy-1-(1H-imidazo1-4-yl)-2-methylpropyl]-N,N-dimethyl-2-naphthamide 337523-06-5P, 1-(1H-Imidazo1-4-yl)-2-methyl-1-[6-(1-pyrrolidinylcarbonyl)-2-naphthyl]-1-propanol 337523-11-2P, 6-[1-Hydroxy-1-(1H-imidazo1-4-yl)-2-methylpropyl]-N-(1,3-thiazo1-2-yl)-2-naphthamide 337523-16-7P, N-Ethoxy-6-[1-hydroxy-1-(lH-imidazol-4-yl)-2-methylpropy1]-2-naphthamide 337523-20-3P, 6-{1-Hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl}-N-isopropoxy-2-naphthamide 337523-24-7P, N-(2-Hydroxyethyl)-6-{1hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2-naphthamide 337523-32-7P 337523-36-1P 337523-47-4P **337523-61-2P**, (S)-(-)-6-[1-Hydroxy-1-(1H-imidazol-4-y1)-2-methylpropyl]-N-methyl-2-naphthamide **337523-63-4P**, methylpropyl] - n-methyl-2-maphthamide 33/323-33-49, (S) - (-) -N-Ethyl-6-[1-hydroxy-1- (1H-imidazol-4-yl) - 2-methylpropyl] - 2-naphthamide 337523-65-69, (S) - (-) -N-Cyclopropyl-6-[1-hydroxy-1- (1H-imidazol-4-yl) - 2-methylpropyl] - 2-naphthamide 337523-76-99, 1-[5-Chloro-6-(1,3-oxazol-5-yl) - 2-naphthyl] - 1- (1H-imidazol-4-yl) - 2-methyl-1-propanol 337523-62-79, 6-[1-Hydroxy-1-(1H-imidazol-4-yl) - 3-methylbyll - 2-methylpropyll - 1 (1H-imidazol-4-yl) - 3-methylpropyll - 2-methylpropyll - 1 (1H-imidazol-4-yl) - 3-methylpropyll - 2-methylpropyll - 2-methylpropyl methylbutyl]-2-naphthamide 337523-86-1P, 1-(1H-Imidazol-4-yl)-3methyl-1-[6-(lH-1,2,3-triazol-4-yl)-2-naphthyl]-1-butanol337523-94-1P, 1-(iH-Imidazol-4-yl)-3-methyl-1-[6-(1,3-0xazol-5-yl)-2-naphthyl]-1-butanol 337524-00-2P, 1-[6-(4,4-Dimethyl-4,5-dihydro-1,3-0xazol-2-yl)-2-naphthyl]-1-(iH-imidazol-4-yl)-2-methyl-1propanol 337524-05-7P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of imidazolyl naphthalenemethanol steroid C17-20 lyase inhibitors for treatment of breast and prostate cancer)

1H-Imidazole-4-methanol, .alpha.-(6,7-dimethoxy-2-naphthalenyl)-.alpha.-(1-

Absolute stereochemistry. Rotation (-).

methylethyl) -, (.alpha.S) - (9CI) (CA INDEX NAME)

336102-68-2 CAPLUS

2-Naphthalenecarboxylic acid, 6-[1-hydroxy-1-(1H-imidazol-4-yl)-2methylpropyl]-, methyl ester (9CI) (CA INDEX NAME)

ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

337521-70-7 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(1-methylethyl)-.alpha.-[6-(2-thienyl)-2naphthalenyl) - (9CI) (CA INDEX NAME)

337521-74-1 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(1-methylethyl)-.alpha.-[6-(1H-1,2,3-

triazol-4-yl)-2-naphthalenyl}- (9CI) (CA INDEX NAME)

337521-77-4 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(1-methylethyl)-.alpha.-[6-(1H-tetrazol-5yl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)

337521-79-6 CAPLUS

lH-Imidazole-4-methanol, .alpha.-(1-methylethyl)-.alpha.-[6-(1H-pyrazol-4-

yl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & i-Pr & H \\ \downarrow & \downarrow & \downarrow \\ CH & N \end{array}$$

ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

336102-70-6 CAPLUS

CN 2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-yl)-3-methylbutyl]-N-methyl- (9CI) (CA INDEX NAME)

336102-73-9 CAPLUS

2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-yl)propyl]-N-

methyl- (9CI) (CA INDEX NAME)

337521-66-1 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(1-methylethyl)-.alpha.+(6-phenyl-2naphthalenyl) - (9CI) (CA INDEX NAME)

337521-68-3 CAPLUS

1H-Imidazole-4-methanol, .alpha.-[6-(2-furanyl)-2-naphthalenyl]-.alpha.-(1methylethyl) - (9CI) (CA INDEX NAME)

ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

337521-81-0 CAPLUS $l \hbox{H-Imidazole-4-methanol, .alpha.-(1-methylethyl)-.alpha.-(6-(5-oxazolyl)-2-1)} \\$ naphthalenyl] - (9CI) (CA INDEX NAME)

337521-84-3 CAPLUS

2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-y1)-2methylpropyl]-N-methyl- (9CI) (CA INDEX NAME)

337521-86-5 CAPLUS

2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-y1)-2methylpropyl]-N-methoxy- (9CI) (CA INDEX NAME)

337521-89-8 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(1-methylethyl)-.alpha.-naphtho[2,1b]furan-7-yl- (9C1) (CA INDEX NAME)

337521-95-6 CAPLUS

lH-Imidazole-4-methanol, .alpha.-(1,2-dihydronaphtho[2,1-b]furan-7-y1)-

.alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME)

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ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

337522-00-6 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(2,3-dihydro-1H-naphtho[2,1-b]pyran-8-yl).alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME)

337522-09-5 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(2,3-dihydro-1H-naphtho[2,1-b]pyran-8-yl)-.alpha.-methyl- (9CI) (CA INDEX NAME)

337522-10-8 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(2,3-dihydro-1H-naphtho(2,1-b)pyran-8-yl)-.alpha.-ethyl- (9CI) (CA INDEX NAMÉ)

337522-12-0 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(1,2-dihydronaphtho[2,1-b]furan-7-yl)-

.alpha.-methyl- (9CI) (CA INDEX NAME)

ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

337522-33-5 CAPLUS

Acetamide, N-[6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2-naphthalenyl]-, (-)- (9CI) (CA INDEX NAME)

337522-40-4 CAPLUS

Acetamide, N-[6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2-naphthalenyl]-, (-)-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 337522-33-5

CMF C19 H21 N3 O2

Rotation (-).

CM 2

CRN 110-17-8 CMF C4 H4 04

Double bond geometry as shown.

337522-41-5 CAPLUS

2-Naphthalenecarboxamide, N-ethyl-6-(1-hydroxy-1-(1H-imidazol-4-yl)-2methylpropyl] - (9CI) (CA INDEX NAME)

ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

337522-21-1 CAPLUS

lH-Imidazole-4-methanol, .alpha.-(1,2-dihydronaphtho[2,1-b]furan-7-yl)-.alpha.-ethyl- (9CI) (CA INDEX NAME)

(Continued)

337522-31-3 CAPLUS

HH-Imidazole-4-methanol, .alpha.-(6,7-dimethoxy-2-naphthalenyl)-.alpha.-(1-methylethyl)-, (-)-, (2E)-2-butenedicate (1:1) (salt) (9CI) (CA INDEX

CM 1

CRN 336102-55-7

CMF C19 H22 N2 O3

Absolute stereochemistry. Rotation (-).

CRN 110-17-8 CMF C4 H4 Q4

Double bond geometry as shown.

L6 ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

337522-49-3 CAPLUS

2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-yl)-2methylpropyl] -N-(1-methylethyl) - (9CI) (CA INDEX NAME)

337522-53-9 CAPLUS

2-Naphthalenecarboxamide, N-butyl-6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]- (9CI) (CA INDEX NAME)

337522-57-3 CAPLUS

2-Naphthalenecarboxamide, N-cyclopropyl-6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl] - (9CI) (CA INDEX NAME)

337522-61-9 CAPLUS

2-Naphthalenecarboxamide, N-cyclobutyl-6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-

methylpropyl} - (9CI) (CA INDEX NAME)

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L6 ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

337522-64-2 CAPLUS

2-Naphthalenecarboxamide, N-(cyclopropylmethyl)-6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]- (9CI) (CA INDEX NAME)

337522-67-5 CAPLUS

2-Naphthalenecarboxamide, N-cyclopentyl-6-[1-hydroxy-1-(lH-imidazol-4-yl)-2-methylpropyl]- (9C1) (CA INDEX NAME)

337522-69-7 CAPLUS

2-Naphthalenecarboxamide, N-cyclohexyl-6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]- (9CI) (CA INDEX NAME)

337522-72-2 CAPLUS

2-Naphthalenecarboxamide, N-cycloheptyl-6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]- (9CI) (CA INDEX NAME)

ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

337522-88-0 CAPLUS

2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-N,1-dimethyl- (9CI) (CA INDEX NAME)

337522-99-3 CAPLUS

CN 2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-yl)-2methylpropyl]-3-methyl- (9CI) (CA INDEX NAME)

337523-03-2 CAPLUS

2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-y1)-2methylpropyl]-N, N-dimethyl- (9C1) (CA INDEX NAME)

337523-06-5 CAPLUS

Pyrrolidine, 1-[[6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2-naphthalenyl]carbonyl]- (9CI) (CA INDEX NAME)

ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

337522-74-4 CAPLUS

2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]- (9CI) (CA INDEX NAME)

337522-77-7 CAPLUS

2-Naphthalenecarboxamide, 1-chloro-6-[1-hydroxy-1-(1H-imidazol-4-yl)-2methylpropyl] - (9CI) (CA INDEX NAME)

337522-79-9 CAPLUS

2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-1-methyl- (9CI) (CA INDEX NAME)

RN 337522-83-5 CAPLUS

2-Naphthalenecarboxamide, 1-chloro-6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-N-methyl- (9CI) (CA INDEX NAME)

L6 ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

337523-11-2 CAPLUS

2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-y1)-2methylpropyl]-N-2-thiazolyl- (9CI) (CA INDEX NAME)

337523-16-7 CAPLUS

2-Naphthalenecarboxamide, N-ethoxy-6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]- (9CI) (CA INDEX NAME)

337523-20-3 CAPLUS

2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-y1)-2methylpropyl]-N-(1-methylethoxy)- (9CI) (CA INDEX NAME)

337523-24-7 CAPLUS

CN 2-Naphthalenecarboxamide, N-(2-hydroxyethyl)-6-[1-hydroxy-1-(1H-imidazol-4-

yl)-2-methylpropyl]- (9CI) (CA INDEX NAME)

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L6 ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

$$HO-CH_2-CH_2-NH-C$$
 OH
 OH
 OH
 OH

RN 337523-32-7 CAPLUS
CN L-Alanine, N-[[6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2naphthalenyl]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 337523-36-1 CAPLUS
CN D-Alanine, N-[[6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2-naphthalenyl]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 337523-47-4 CAPLUS
CN 2-Naphthalenecarboxamide, 6-(cyclopropylhydroxy-1H-imidazol-4-ylmethyl)-Nmethyl- (9CI) (CA INDEX NAME)

L6 ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 337523-76-9 CAPLUS
CN 1H-Imidazole-4-methanol, .alpha.-{5-chloro-6-{5-oxazoly1}-2-naphthalenyl}.alpha.-{1-methylethyl}- (9CI) {CA INDEX NAME}

RN 337523-82-7 CAPLUS
CN 2-Naphthalenecarboxamide, 6-[1-hydroxy-1-(1H-imidazol-4-yl)-3-methylbutyl](9CI) (CA INDEX NAME)

RN 337523-86-1 CAPLUS
CN lH-Imidazole-4-methanol, .alpha.-(2-methylpropyl)-.alpha.-[6-(1H-1,2,3-triazol-4-yl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 337523-94-1 CAPLUS
CN 1H-Imidazole-4-methanol, .alpha.-(2-methylpropyl)-.alpha.-(6-(5-oxazolyl)-2-naphthalenyl)- (9CI) (CA INDEX NAME)

L6 . ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 337523-61-2 CAPLUS
CN 2-Naphthalenecarboxamide, 6-[(1S)-1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 337523-63-4 CAPLUS
CN 2-Naphthalenecarboxamide, N-ethyl-6-((15)-1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 337523-65-6 CAPLUS
CN 2-Naphthalenecarboxamide, N-cyclopropyl-6-[(1S)-1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L6 ANSWER 10 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 337524-00-2 CAPLUS
CN 1H-Imidazole-4-methanol, .alpha.-[6-(4,5-dihydro-4,4-dimethyl-2-oxazolyl)-2-naphthalenyl]-.alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & i - P r & H \\ & \downarrow & & \downarrow \\ Me & & OH & N \end{array}$$

RN 337524-05-7 CAPLUS
CN 2-Naphthalenecarboxamide, 6-[(1S)-1-hydroxy-1-(1H-imidazol-4-yl)propyl]-N-methyl-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 336103-03-8 CMF C18 H19 N3 02

Absolute stereochemistry. Rotation (-).

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

CMF C4 H4 04

Е СО2Н

REFERENCE COUNT:

6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L6 ANSWER 11 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 2001:12424 CAPLUS DOCUMENT NUMBER: 134:86245 TITLE: Preparation of imidazoles as selective agonists at .alpha.2b or .alpha.2b/.alpha.2c adrenergic receptors. Chow, Ken; Gil, Daniel W.; Burke, James A.; Harcourt, INVENTOR(S): Dale A.; Garst, Michael E.; Wheeler, Larry A.; Munk, Stephen A. PATENT ASSIGNEE(S): Allergan Sales, Inc., USA SOURCE: PCT Int. Appl., 145 pp. CODEN: PIXXD2 DOCUMENT TYPE: Patent LANGUAGE: English

PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE WO 2001000586 Αì 20010104 WO 2000-US15795 20000608 W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, FT, RO, RU, SD, SE, SG, SI, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

1104407 A1 20010606 EP 2000-939699 20000609

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

2002156076 A1 20021024 US 2001-948001 20010906

APPLN. INFO:: EP 1104407 US 2002156076 PRIORITY APPLN. INFO .: US 1999-329752 A 19990610 US 1997-985347 B2 19971204

US 1998-205597

WO 2000-US15795 W 20000608

B2 19981204

US 2000-679919 A1 20001005 OTHER SOURCE(S): MARPAT 134:86245

FAMILY ACC. NUM. COUNT:

Title compds. {I; dotted lines = optional double bonds; R = H, alkyl; X = S, CHR1; R1 = H, alkyl, nuil; Y = O, N, S, [C(R1)n]y, CH:CH, Y1CH2; Y = 1-3; n = 1, 2; R2 = H, alkyl, halo, OH, alkoxy, alkenyl, acyl, alkynyl, etc.; R3R = H, alkyl, halo, alkenyl, acyl, alkynyl, etc.; R3R4 = atoms to form (unsatd.) (heterocyclic) ring], were prepd. Thus, 1-(dimethylsulfamoyl)imidazole in THF at -78.degree. was treated with BuLi and tert-butyldimethylsilyl chloride followed by warming to room temp., stirring oversight, cooled to -20 degree. stirring overnight, cooled to -20.degree., and treatment with BuLi and

ANSWER 11 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

$$\text{MeO} \longrightarrow \text{CH}_2 \longrightarrow \text{H}_N$$

HCl

226571-02-4 CAPLUS

1(2H) -Naphthalenone, 3,4,5,6,7,8 -hexahydro-2-(1H-imidazol-4-ylmethyl)-(CA INDEX NAME)

lH-Imidazole, 4-((1,2,3,4,5,6,7,8-octahydro-2-naphthalenyl)methyl]- (9CI)

157058-44-1 157058-52-1 226571-13-7 226571-14-8 226571-25-1 226571-26-2 226571-35-3 226571-36-4 226571-37-5

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES

(prepn. of imidazoles as selective agonists at .alpha.2b or .alpha.2b/.alpha.2c adrenergic receptors) 157058-44-1 CAPLUS

1(2H)-Naphthalenone, 3,4-dihydro-2-(lH-imidazol-4-ylmethyl)- (9CI) (CA

157058-52-1 CAPLUS

1H-Imidazole, 4-[(1,2,3,4-tetrahydro-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

ANSWER 11 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN 3-thiophenecarboxaldehyde followed by warming to room temp. and stirring overnight to give 2-(tert-butyldimethylsily1)-5-(hydroxythiophen-2ylmethyl)imidazole-1-sulfonic acid dimethylamide. This was treated sequentially with Bu4NF, Et3SiH/CF3CO2H/CH2C12, and aq. HCl to give 4(5)-thiophen-3-ylmethyl-1H-imidazole. Tested I as eyedrops at 0.03-1% reduced intraocular pressure in cynomolgus monkeys by 12.4-33% and showed no sedative activity. 157058-47-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of imidazoles as selective agonists at .alpha.2b or

.alpha.2b/.alpha.2c adrenergic receptors) 157058-47-4 CAPLUS

1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-7-methoxy-(9CI) (CA INDEX NAME)

157058-55-4P 226570-89-4P 226571-02-4P ΙT

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of imidazoles as selective agonists at .alpha.2b or .alpha.2b/.alpha.2c adrenergic receptors)

157058-55-4 CAPLUS

1H-Imidazole, 4-[(1,2,3,4-tetrahydro-7-methoxy-2-naphthalenyl)methyl]-(9CI) (CA INDEX NAME)

$$CH_2 \xrightarrow{H}_N$$

226570-89-4 CAPLUS

 $1 \\ H-Imidazole, \ 4-[(1,2,3,4-tetrahydro-7-methoxy-2-naphthalenyl) methyl]-,$ monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 11 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

226571-13-7 CAPLUS

1H-Imidazole, 4-[[(2S)-1,2,3,4-tetrahydro-2-naphthalenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

226571-14-8 CAPLUS

1H-Imidazole, 4-[[(2R)-1,2,3,4-tetrahydro-2-naphthalenyl]methyl]- (9CI)

Absolute stereochemistry

226571-25-1 CAPLUS

1H-Imidazole, 4-[(1,2,3,4-tetrahydro-4-methyl-2-naphthalenyl)methyl]-CN (9CI) (CA INDEX NAME)

226571-26-2 CAPLUS

1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-4-methyl-(9CI) (CA INDEX NAME)

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ANSWER 11 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

226571-35-3 CAPLUS 1H-Imidazole, 4-[(1,2,3,4-tetrahydro-4,4-dimethyl-2-naphthalenyl)methyl] (9CI) (CA INDEX NAME)

226571-36-4 CAPLUS 1H-Imidazole, 4-[{1,2,3,4-tetrahydro-7-methyl-2-naphthalenyl}methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Me
$$CH_2$$
 N

• HCl

226571-37-5 CAPLUS 1 (2H) -Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-7-methyl-(9CI) (CA INDEX NAME)

226571-57-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of imidazoles as selective agonists at .alpha.2b or .alpha.2b/.alpha.2c adrenergic receptors)

L6 ANSWER 12 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN 2000:911226 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

Process for the preparation of 4-alkanoylimidazole derivatives and 1-(2-naphthyl)-1-(1H-imidazol-4yl) alkanol derivatives Kawakami, Jun-ichi

Takeda Chemical Industries, Ltd., Japan

INVENTOR(S): PATENT ASSIGNEE (S):

PCT Int. Appl., 39 pp.

SOURCE:

CODEN: FIXXD2 DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

OTHER SOURCE(S):

APPLICATION NO. DATE PATENT NO. KIND DATE 20001228 WO 2000-JP4036 20000621 WO 2000078727 Al AE, AG, AL, AM, AU, AZ, BA, FB, BG, BR, BY, BZ, CA, CN, CR, CU, CZ, DM, DZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG JP 2000-191081 20000621 EP 2000-940770 20000621 JP 2001064264 A2 20010313 A1 20020403 EP 1193258 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO JP 1999-175070 A 19990622 WO 2000-JP4036 W 20000621 PRIORITY APPLN. INFO .: CASREACT 134:56671; MARPAT 134:56671

An industrially advantageous process for the prepn. of compds. of general formula (I; wherein the ring A is an optionally substituted imidazole ring: R is an optionally substituted hydrocarbon group or a heterocyclic

ANSWER 11 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

226571-57-9 CAPLUS RN

1-Naphthalenol, 1,2,3,4-tetrahydro-2-(lH-imidazol-4-ylmethyl)-7-methoxy-(9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 12 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) group; and R1, R2, R3, R4, R5, R6, and R7 are each hydrogen, optionally substituted hydrocarbyl, OH, SH, NH2, acyl, halogeno, or the like) comprises addn. reaction of 4-cyanoimidazole (II; the ring A is same as above) with R-M1 (R is same as above; M1 = alkali metal, Mg-Y1; Y1 = halo) to give 4-acylimidazole (III; R and ring A are same as above), followed by addn. reaction of III with naphthalene alkali metals (IV; R1 - R7 are = same as above; M2 is alkali metal, Mg-Y2; Y2 is halo). This process is reduced in the no. of steps, attains a high yield, and process is reduced in the no. of steps, attains a high yield, and dispenses with the use of a heavy metal compd. The compds. I exhibit a steroid C17-C20 lyase inhibitory activity (no data). Thus, a soln. of 42.7 g 4-cyanoimidazole in 500 mL THF was added dropwise to a 1.1. M soln. of isopropylmagnesium bromide in THF (1.4 L) over a period of 30 min, stirred at 15-25.degree., treated dropwise with 10% aq. H2504, stirred for 30 min, neutralized to pH 8 with 30 aq. NaOH, and extd. with EtoAc (300 L) the site (30% L) (11 initiated 1.4 m) (21 moth) (12 moth) (12 moth) (12 moth) (13 mo .times. 2) to give 82% 1-(1H-imidazol-4-yl)-2-methyl-1-propanone (V). 2-Bromo-6-methoxynaphthalene (5.15 g) was added dropwise to a mixt. of 0.55 g and 3 mg iodine in THF at 50.degree. and stirred at 15-25.degree. for 1.5 h, followed by adding dropwise a soln. of 1 g V in THF, and the resulting mixt. was stirred at 15-25.degree. for 8 h to give, after workup, 84% 1-(lH-imidazol-4-yl)-1-(6-methoxynaphthalen-2-yl)-2-

247173-05-3P RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)

(preph. of 4-alkanovlimidazole derivs. and .alpha.-(2-naphthyl)-.alpha.-(lH-imidazolyl) alkanol derivs. by addn, reaction of cyanoimidazoles with alkylmagnesium bromides followed by naphthylmagnesium bromide)

247173-05-3 CAPLUS 1H-Imidazole-4-methanol, .alpha.-(6-methoxy-2-naphthalenyl)-.alpha.-(1methylethyl) - (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Page 30 01/13/2004 L6 ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1999:691084 CAPLUS DOCUMENT NUMBER: 131:299449 Preparation of azolylmethylnaphthalenes and related compounds as steroid C17, 20-lyase inhibitors. Tasaka, Akihiro: Ojida, Akio: Kaku, Tomohiro: Kusaka, INVENTOR (S): Masami: Yamaoka, Masuo Takeda Chemical Industries, Ltd., Japan PATENT ASSIGNEE(S): PCT Int. Appl., 131 pp. SOURCE: CODEN: PIXXD2 DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. APPLICATION NO. DATE KIND DATE WO 9954309 A1 19991028 WO 1999-JP2143 19990422 W: AE, AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, S1, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG 19991028 CA 1999-2328973 CA 2328973 AA 19990422 AU 9935346 AU 1999-35346 JP 2000007658 20000111 JP 1999-114398 EP 1073640 A1 20010207 EP 1999-917102 19990422 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI US 6573289 20030603 В1 US 2000-673591 20001018 US 2003236274 20030522 A1 20031225 US 2003-443379 JP 1998-113801 A 19980423 PRIORITY APPLN. INFO .: US 2000-673591 A3 20001018 OTHER SOURCE(S): MARPAT 131:299449 Title compds. [I; Al = (substituted) imidazolyl, thiazolyl, oxazolyl, pyridyl; R11 = H, (substituted) hydrocarbyl, monocyclic heteroaryl; R21 = H, (substituted) alkyl; R3-R9 = H, (substituted) hydrocarbyl, OH, SH, amino, acyl, halo; R21 = (substituted) alkyl), and salts or prodrugs thereof, were prepd. Thus, 2-bromo-6-methoxynaphthalene in THF at -78.degree. was treated with BuLi and then with 4-formyl-1-trityl-1H-ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) 247173-07-5 CAPLUS RN 1H-Imidazole-4-methanol, .alpha.-(6-methoxy-2-naphthalenyl)-.alpha.-(trifluoromethyl) - (9CI) (CA INDEX NAME) 247173-09-7 CAPLUS 1H-Imidazole-4-methanol, .alpha.-cyclopropyl-.alpha.-(6-methoxy-2naphthalenyl)-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME) CM 1

CRN 247173-08-6 CMF C18 H18 N2 O2

CM

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

247173-11-1 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(1,1-dimethylethyl)-.alpha.-(6-methoxy-2naphthalenyl) -, (2E) -2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CRN 247173-10-0 CMF C19 H22 N2 O2

ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) imidazole to give (6-methoxynaphthalen-2-yl) (1-trityl-1H-imidazol-4yl)methanol. The product was refluxed with MnO2 in CHC13 to give the ketone, which was detritylated with HCO2H in THF to give (lH-imidazol-4-yl)(6-methoxynaphthalen-2-yl) ketone. The latter in THF at -10.degree. was treated with Me2CHMgBr in THF to give 1-(1H-imidazol-4-yl) 1-(6-methoxynaphthalen-2-yl)-2-methyl-1-propanol. This inhibited rat steroid C17,20-lyase with IC50 = 33 nM. I drug formulations are given. 247173-05-3P 247173-06-4P 247173-07-5P 247173-09-7P 247173-11-1P 247173-12-2P 247173-13-3P 247173-14-4P 247173-17-7P 247173-18-8P 247173-19-9P 247173-20-2P 247173-21-3P 247173-22-4P 247173-24-6P 247173-25-7P 247173-26-8P 247173-27-9P 247173-28-0P 247173-29-1P 247173-30-4P 247173-31-5P 247173-32-6P 247173-33-7P 247173-34-8P 247173-35-9P 247173-36-0P 247173-37-1P 247173-38-2P 247173-39-3P 247173-40-6P 247173-41-7P 247173-42-8P 247173-43-9P 247173-44-0P 247173-45-1P 247173-46-2P 247173-47-3P 247173-48-4P 247173-49-5P 247173-50-8P 247173-51-9P 247173-52-0P 247173-53-1P 247173-54-2P 247173-55-3P 247173-56-4P 247173-57-5P 247173-58-6P 247173-59-7P 247173-60-0P 247173-61-1P 247173-62-2P 247173-63-3P 247173-64-4P 247173-65-5P 247173-66-6P 247173-68-8P 247173-69-9P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of azolylmethylnaphthalenes and related compds. as steroid C17,20-lyase inhibitors) 247173-05-3 CAPLUS 1H-Imidazole-4-methanol, .alpha.-(6-methoxy-2-naphthalenyl)-.alpha.-(1methylethyl) - (9CI) (CA INDEX NAME) 247173-06-4 CAPLUS (9CI) (CA INDEX NAME)

1H-Imidazole-4-methanol, .alpha.-(6-methoxy-2-naphthalenyl)-.alpha.-methyl-

ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

247173-12-2 CAPLUS 3-Pyridinemethanol, .alpha.-1H-imidazol-4-yl-.alpha.-(6-methoxy-2-naphthalenyl)- (9CI) (CA INDEX NAME)

247173-13-3 CAPLUS 4-Pyridinemethanol, .alpha.-lH-imidazol-4-yl-.alpha.-{6-methoxy-2naphthalenyl) - (9CI) (CA INDEX NAME)

247173-14-4 CAPLUS CN 1H-Imidazole-4-methanol, .alpha.-(6-methoxy-2-naphthalenyl)-.alpha.-phenyl-(9CI) (CA INDEX NAME)

247173-17-7 CAPLUS RN 1H-Imidazole-4-methanol, .alpha.-(5-fluoro-6-methoxy-2-naphthalenyl)-CN .alpha.-(1-methylethyl)- (9C1) (CA INDEX NAME)

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L6 ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 247173-18-8 CAPLUS
CN 1H-Imidazole-4-methanol, .alpha.-ethyl-.alpha.-(6-methoxy-2-naphthalenyl)(9CI) (CA INDEX NAME)

RN 247173-19-9 CAPLUS
CN 1H-Imidazole-4-methanol, .alpha.-(6-methoxy-2-naphthalenyl)-.alpha.-(2-methylpropyl)-`(9CI) (CA INDEX NAME)

RN 247173-20-2 CAPLUS
CN 1H-Imidazole-4-methanol, .alpha.-(6-methoxy-2-naphthalenyl)-.alpha.-propyl(9CI) (CA INDEX NAME)

RN 247173-21-3 CAPLUS
CN 1H-Imidazole-4-methanol, .alpha.-cyclopentyl-.alpha.-(6-methoxy-2-naphthalenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued

RN 247173-27-9 CAPLUS
CN 1H-Imidazole, 4-[(6-methoxy-2-naphthalenyl)(1-methylethoxy)methyl]- (9CI)
(CA INDEX NAME)

RN 247173-28-0 CAPLUS
CN 1H-Imidazole-4-methanol, .alpha.-(6-methoxy-2-naphthalenyl)-.alpha.-(1-methylethenyl)- (9CI) (CA INDEX NAME)

RN 247173-29-1 CAPLUS
CN 1H-Imidazole-4-methanol, .alpha.-(5-chloro-6-methoxy-2-naphthalenyl).alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 247173-30-4 CAPLUS
CN 1H-Imidazole-4-methanol, .alpha.-[5-[1-[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethyl]-6-methoxy-2-naphthalenyl]-.alpha.(1-methylethyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 247173-22-4 CAPLUS
CN 1H-Imidazole-4-methanol, .alpha.~(6-hydroxy-2-naphthalenyl)-.alpha.~(1-methylethyl)- (9CI) {CA INDEX NAME}

RN 247173-24-6 CAPLUS
CN 1H-Imidazole, 4-[1-methoxy-1-(6-methoxy-2-naphthaleny1)ethy1]- (9CI) (CA INDEX NAME)

RN 247173-25-7 CAPLUS
CN 1H-Imidazole, 4-[1-methoxy-1-(6-methoxy-2-naphthaleny1)-2-methylpropyl](9CI) (CA INDEX NAME)

RN 247173-26-8 CAPLUS
CN 1H-Imidazole, 4-[methoxy(6-methoxy-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

L6 ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 247173-31-5 CAPLUS
CN 1,6-Naphthalenedimethanol, .alpha.6-1H-imidazol-4-yl-2-methoxy-.alpha.1-methyl-.alpha.6-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 247173-32-6 CAPLUS
CN 1H-Imidazole-4-methanol, .alpha.-(1-methylethyl)-.alpha.-(6-(phenylmethoxy)-2-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 247173-33-7 CAPLUS
CN 1H-Imidazole-4-methanol, .alpha.-[6-methoxy-5-(1-methyletheny1)-2-naphthalenyl]-.alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 247173-34-8 CAPLUS CN 1H-Imidazole-4-methanol, .alpha.-[6-methoxy-5-(1-methylethyl)-2-

Page 32 01/13/2004

ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) naphthalenyl] -. alpha. - (1-methylethyl) - (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} i-Pr & H \\ \hline \\ Pr-i & H \\ \hline \\ C & N \\ \end{array}$$

247173-35-9 CAPLUS

Propanoic acid, 2,2-dimethyl-, [[6-[1-hydroxy-1-(1H-imidazol-4-yl)-2methylpropyl]-2-naphthalenyl]oxy]methyl ester (9CI) (CA INDEX NAME)

247173-36-0 CAPLUS

1H-Imidazole-4-methanol, .alpha.-[6-(1-methylethoxy)-2-naphthalenyl]-.alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME)

247173-37-1 CAPLUS RN

1H-Imidazole-4-methanol, .alpha.-(1-methylethyl)-.alpha.-(6-propoxy-2-CN naphthalenyl) - (9CI) (CA INDEX NAME)

247173-38-2 CAPLUS RN

Propanoic acid, 2,2-dimethyl-, 6-[1-hydroxy-1-(1H-imidazo1-4-yl)-2-methylpropyl]-2-naphthalenyl ester (9CI) (CA INDEX NAME)

ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

247173-43-9 CAPLUS

lH-Imidazole-4-methanol, .alpha.-(5,6-dimethoxy-2-naphthalenyl)-.alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME)

4/1/3-44-0 CAPLUS

IH-Imidazole-4-methanol, .alpha.-(6-hydroxy-7-methoxy-2-naphthalenyl).alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME)

247173-45-1 CAPLUS

1,6-Naphthalenedimethanol, .alpha.6-1H-imidazol-4-yl-2-methoxy-.alpha.6-(1methylethyl) - (9CI) (CA INDEX NAME)

247173-46-2 CAPLUS

1H-Imidazole-4-methanol, .alpha.-{6-methoxy-5-(methoxymethyl)-2-naphthalenyl}-.alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME) CN

L6 ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

247173-39-3 CAPLUS

lH-Imidazole-4-methanol, .alpha.-[6-(2-methoxyethoxy)-2-naphthalenyl]-.alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME) CN

$$\underset{\mathsf{MeO-CH}_2-\mathsf{CH}_2-\mathsf{O}}{\overset{\mathsf{i-Pr}}{\underset{\mathsf{OH}}{\overset{\mathsf{I-N}}{\underset{\mathsf{N}}{\bigvee}}}}} \overset{\mathsf{H}}{\underset{\mathsf{N}}{\underset{\mathsf{N}}{\bigvee}}}$$

247173-40-6 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(6-ethoxy-2-naphthalenyl)-.alpha.-(1methylethyl) - (9CI) (CA INDEX NAME)

247173-41-7 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(6,7-dimethoxy-2-naphthalenyl)-.alpha.-(1-methylethyl)- (9C1) (CA INDEX NAME) CN

 $1 \\ H-Imidazole-4-methanol, \ .alpha.-(6-methoxy-5-methyl-2-naphthalenyl)-1 \\ H-Imidazole-4-methyl-2-meth$.alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

247173-47-3 CAPLUS

IH-Imidazole-4-methanol, .alpha.-(5-ethyl-6-methoxy-2-naphthalenyl).alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME)

247173~48-4 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(5-ethenyl-6-methoxy-2-naphthalenyl)-.alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME)

247173-49-5 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(5-bromo-6-methoxy-2-naphthalenyl)-.alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME)

247173-50-8 CAPLUS

1H-Imidazole-4-methanol, .alpha.-[6-(fluoromethoxy)-2-naphthalenyl]-.alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME) CN

Page 33 01/13/2004

L6 ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

247173-51-9 CAPLUS 1H-Imidazole-4-methanol, .alpha.-(6-methoxy-5,7-dimethyl-2-naphthalenyl)-CN .alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME)

247173-52-0 CAPLUS 1H-Imidazole-4-methanol, .alpha.-(6-bromo-2-naphthalenyl)-.alpha.-(1methylethyl) - (9CI) (CA INDEX NAME)

247173-53-1 CAPLUS 1H-Imidazole-4-methanol, .alpha.-(6-amino-2-naphthalenyl)-.alpha.-(1methylethyl) - (9CI) (CA INDEX NAME)

247173-54-2 CAPLUS Acetamide, N-[6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2naphthalenyl] - (9CI) (CA INDEX NAME)

L6 ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

247173-59-7 CAPLUS Ethanone, 1-[6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2naphthalenyl]- (9CI) (CA INDEX NAME)

247173-60-0 CAPLUS 1-Propanone, 1-[6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2naphthalenyl] - (9CI) (CA INDEX NAME)

247173-61-1 CAPLUS 1-Propanone, 1-[6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2-naphthalenyl]-2-methyl- (9CI) (CA INDEX NAME) CN

247173-62-2 CAPLUS 1H-Imidazole-4-methanol, .alpha.-(6-ethyl-2-naphthalenyl)-.alpha.-(1methylethyl) - (9CI) (CA INDEX NAME)

L6 ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

247173-55-3 CAPLUS

Urea, N'-[6-[1-hydroxy-1-(1H-imidazol-4-yl)-2-methylpropyl]-2naphthalenyl]-N, N-dimethyl- (9CI) (CA INDEX NAME)

247173-56-4 CAPLUS

N'-methyl- (9CI) (CA INDEX NAME)

247173-57-5 CAPLUS

Methanesulfonamide, N-[6-[1-hydroxy-1-(1H-imidazol-4-y1)-2-methylpropy1]-2naphthalenyl] - (9CI) (CA INDEX NAME)

247173-58-6 CAPLUS

2,6-Naphthalenedimethanol, .alpha.-1H-imidazol-4-yl-.alpha.-(1methylethyl) - (9CI) (CA INDEX NAME)

L6 ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

247173-63-3 CAPLUS RN 1H-Imidazole-4-methanol, .alpha.-(1-methylethyl)-.alpha.-(6-methyl-2naphthalenyl) - (9CI) (CA INDEX NAME)

247173-64-4 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(6-ethynyl-2-naphthalenyl)-.alpha.-(1methylethyl) - (9CI) (CA INDEX NAME)

247173-65-5 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(1-methylethyl)-.alpha.-[6-(methylthio)-2-naphthalenyl]- (9CI) (CA INDEX NAME) CN

247173-66-6 CAPLUS RN

1H-Imidazole-4-methanol, .alpha.-(6-methoxy-1-methyl-2-naphthalenyl)-.alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME) CN

247173-68-8 CAPLUS

1H-Imidazole-4-methanol, .alpha.-(1-methylethyl)-.alpha.-(6-propyl-2-

naphthalenyl) - (9CI) (CA INDEX NAME)

Page 34 01/13/2004

L6 ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

247173-69-9 CAPLUS RN 1H-Imidazole-4-methanol, .alpha.-(1-methylethyl)-.alpha.-[6-(1-CN methylethyl) - 2-naphthalenyl] - (9CI) (CA INDEX NAME)

247174-67-0 ΙT

RL: RCT (Reactant); RACT (Reactant or reagent) (prepn. of azolylmethylnaphthalenes and related compds. as steroid C17,20-lyase inhibitors)

247174-67-0 CAPLUS Methanone, (5-fluoro-6-methoxy-2-naphthalenyl)-1H-imidazol-4-yl- (9CI) (CA INDEX NAME)

247173-72-4P 247173-89-3P 247173-95-1P 247174-00-1P 247174-01-2P 247174-05-6P 247174-12-5P 247174-17-0P 247174-24-9P 247174-25-0P 247174-26-1P 247174-35-2P 247174-36-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of azolylmethylnaphthalenes and related compds. as steroid C17, 20-lyase inhibitors) 247173-72-4 CAPLUS

Methanone, 1H-imidazol-4-yl(6-methoxy-2-naphthalenyl)- (9CI) (CA INDEX NAME)

ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

247174-05-6 CAPLUS Methanone, lH-imidazol-4-yl[6-methoxy-5-(1-methylethenyl)-2-naphthalenyl]-(9CI) (CA INDEX NAME)

(Continued)

247174-12-5 CAPLUS RN Methanone, (6,7-dimethoxy-2-naphthalenyl)-1H-imidazol-4-yl- (9CI) (CA

INDEX NAME)

247174-17-0 CAPLUS RN

1H-Imidazole-4-methanol, .alpha.-[6-[[(1,1-dimethylethyl)dimethyleilyl]oxy]-2-naphthalenyl]-.alpha.-(1-methylethyl)- (9CI) (CA INDEX NAME)

247174-24-9 CAPLUS

1H-Imidazole-4-methanol, .alpha.-[7-methoxy-6-(phenylmethoxy)-2naphthalenyl] - (9CI) (CA INDEX NAME)

ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

247173-89-3 CAPLUS RNMethanone, 1H-imidazol-4-yl-2-naphthalenyl- (9CI) (CA INDEX NAME) CN

247173-95-1 CAPLUS

Methanone, (5-chloro-6-methoxy-2-naphthaleny1)-1H-imidazol-4-yl- (9CI) (CA INDEX NAME)

247174-00-1 CAPLUS Methanone, [5-[1-[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethyl]-6-methoxy-2-naphthalenyl]-1H-imidazol-4-yl- (9CI) (CA INDEX NAME)

247174-01-2 CAPLUS

Methanone, lH-imidazol-4-yl[6-(phenylmethoxy)-2-naphthalenyl]- (9CI) (CA INDEX NAME)

ANSWER 13 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

247174-25-0 CAPLUS

Methanone, 1H-imidazol-4-yl[7-methoxy-6-(phenylmethoxy)-2-naphthalenyl]-CN (9CI) (CA INDEX NAME)

247174-26-1 CAPLUS

1H-Imidazole-4-methanol, .alpha.-[7-methoxy-6-{phenylmethoxy}-2naphthalenyl] -. alpha. - (1-methylethyl) - (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & i\text{-Pr} & H \\ \hline & I & N \\ \hline & OH & N \\ \end{array}$$

247174-35-2 CAPLUS

CN 1H-Imidazole-4-methanol, .alpha.-(6-methoxy-5,7-dimethyl-2-naphthalenyl)-(9CI) (CA INDEX NAME)

RN 247174-36-3 CAPLUS

Methanone, 1H-imidazol-4-yl(6-methoxy-5,7-dimethyl-2-naphthalenyl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Page 35 01/13/2004

L6 ANSWER 14 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN 1999:375530 CAPLUS ACCESSION NUMBER: DOCUMENT NUMBER: 131:19013 Preparation of .alpha.2B and .alpha.2C adrenoceptor TITLE: agonists INVENTOR(5): Chow, Ken: Gil, Daniel W.; Burke, James A.; Harcourt, Dale A.; Garst, Michael E.; Wheeler, Larry A.; Munk, Stephen A. Allergan Sales, Inc., USA PATENT ASSIGNEE(S): PCT Int. Appl., 121 pp. CODEN: PIXXD2 SOURCE: DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: 4 PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE WO 9928300 19990610 WO 1998-US25669 19981203 W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG 334 AA 19990610 CA 1998-2312334 19981203 CA 2312334 AU 9918025 19990616 AU 1999-18025 19981203 AU 744798 20020307 EP 1036065 Al 20000920 EP 1998-962883 19981203 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI BR 9813381 20001003 BR 1998-13381 19981203 JF 2001524542 19981203 Т2 20011204 JP 2000-523194 NZ 504667 20030328 NZ 1998-504667 19981203 A NO 2000002773 20000802 NO 2000-2773 20000530 20010906 US 2002156076 A1 20021024 US 2001-948001 PRIORITY APPLN. INFO .: US 1997-985347 A 19971204 WO 1998-US25669 W 19981203 US 1998-205597 B2 19981204 US 1999-329752 B3 19990610 US 2000-679919 A1 20001005 OTHER SOURCE(S): MARPAT 131:19013 Title compds. of diverse structural type were prepd. Thus, 7-methoxy-1-tetralone was condensed with 1-dimethylsulfamoyl-2-tert-butyldimethylsilyl-5-imidazolecarboxaldehyde (prepn. given) and the product converted in 3 steps to 4(5)-(7-methoxy-1,2,3,4-tetrahydronaphth-2ylmethyl)-1H-imidazole. Data for biol. activity of title compds. were given. 157058-44-1P 157058-47-4P 157058-52-1P 157058-55-4P 226570-89-4P 226571-02-4P

IT 157058-44+1P 157058-47-4P 157058-52-1P 157058-55-4P 226570-89-4P 226571-02-4P 226571-05-7P 226571-13-7P 226571-14-8P 226571-25-1P 226571-26-2P 226571-35-3P 226571-35-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

L6 ANSWER 14 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Co

$$\mathsf{MeO} \longrightarrow \mathsf{CH}_2 \longrightarrow \mathsf{H}_N$$

• HCl

RN 226571-02-4 CAPLUS

CN 1(2H)-Naphthalenone, 3,4,5,6,7,8-hexahydro-2-(1H-imidazol-4-ylmethyl)-(9CI) (CA INDEX NAME)

RN 226571-05-7 CAPLUS

CN lH-Imidazole, 4-[(1,2,3,4,5,6,7,8-octahydro-2-naphthalenyl)methyl]- (9CI)

RN 226571-13-7 CAPLUS

TN 1H-Imidazole, 4-[[(2S)-1,2,3,4-tetrahydro-2-naphthalenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 226571-14-0 CAPLUS
CN lH-Imidazole, 4-[[(2R)-1,2,3,4-tetrahydro-2-naphthalenyl]methyl]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 14 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of .alpha.2B and .alpha.2C adrenoceptor agonists)
RN 157058-44-1 CAPLUS

CN 1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)- (9CI) (CA INDEX NAME)

RN 157058-47-4 CAPLUS CN 1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-7-methoxy-(9CI) (CA INDEX NAME)

RN 157058-52-1 CAPLUS
CN 1H-Imidazole, 4-{(1,2,3,4-tetrahydro-2-naphthalenyl)methyl]- (9CI) (CA

RN 157058-55-4 CAPLUS
CN 1H-Imidazole, 4-[(1,2,3,4-tetrahydro-7-methoxy-2-naphthalenyl)methyl](9CI) (CA INDEX NAME)

RN 226570-89-4 CAPLUS
CN 1H-Imidazole, 4-[(1,2,3,4-tetrahydro-7-methoxy-2-naphthalenyl)methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

L6 ANSWER 14 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 226571-25-1 CAPLUS
CN 1H-Imidazole, 4-[(1,2,3,4-tetrahydro-4-methyl-2-naphthalenyl)methyl}(9CI) (CA INDEX NAME)

RN 226571-26-2 CAPLUS CN 1(2H)-Naphthalenone, 3,4-dihydro-2-{1H-imidazol-4-ylmethyl}-4-methyl-(9CI) (CA INDEX NAME)

RN 226571-35-3 CAPLUS
CN 1H-Imidazole, 4-[(1,2,3,4-tetrahydro-4,4-dimethyl-2-naphthalenyl)methyl](9CI) (CA INDEX NAME)

RN 226571-36-4 CAPLUS
CN lH-Imidazole, 4-[(1,2,3,4-tetrahydro-7-methyl-2-naphthalenyl)methyl]-,
monohydrochloride (9CI) (CA INDEX NAME)

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ANSWER 14 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

Me
$$CH_2$$
 N

HC1

226571-37-5 CAPLUS 1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-7-methyl-(CA INDEX NAME)

226571-43-3 CAPLUS 1(2H)-Naphthalenone, 3,4,5,6,7,8-hexahydro-2-(1H-imidazol-4-ylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

$$\bigcap_{N}^{\circ} \operatorname{CH}_{2} - \bigcap_{N}^{H}$$

HC1

226571-55-7 CAPLUS 1H-Imidazole, 4-[(1,2,3,4,5,6,7,8-octahydro-2-naphthalenyl)methyl]-, (2E) -2-butenedioate (2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 226571-05-7 CMF C14 H20 N2

L6 ANSWER 15 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1999:244636 CAPLUS

DOCUMENT NUMBER: TITLE:

130:252360 Preparation of dihydronaphthalene compounds

Hartmann, Rolf Wolfgang, Wachall, Bertil, Yoshihama, Makoto, Nakakoshi, Masamichi, Nomoto, Shin, Ikeda, Yoshikazu

PATENT ASSIGNEE(S): SOURCE:

Yukijirushi Nyugyo Kabushiki Kaisha, Japan

PCT Int. Appl., 70 pp. CODEN: PIXXD2

DOCUMENT TYPE:

INVENTOR(S):

Patent Japanese

LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. WO 9918075

KIND DATE APPLICATION NO. DATE WO 1998-JP4426 19981001 A1 19990415 W: AU, CA, CN, FI, HU, IL, JP, KR, MX, NO, NZ, RU, US RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE ZA 9808954 19990412 ZA 1998-8954 19981001 AU 9892810 Α1 19990427 AU 1998-92810 19981001 AU 743405 B2 20020124 EP 1028110 20000816 EP 1998-945556 19981001 CH, DE, DK, ES, NZ 501822 20011221 NZ 1998-501822 19981001 RU 2203890 C2 20030510 RU 1999-127323 19981001 CN 1117732 20030813 CN 1998-808436 19981001 FI 2000000207 20000201 FI 2000-207 20000201 NO 2000001289 20000310 NO 2000-1289 20000310 A US 2002032211 20020314 US 2001-866179 20010525 US 6559157 В2 20030506 JP 1997-284263 A 19971002 WO 1998-JP4426 W 19981001 PRIORITY APPLN. INFO.: WO 1998-JP4426

US 1999-424126 B1 19991117 OTHER SOURCE(S): MARPAT 130:252360

Dihydronaphthalene compds. I (R1 = H, OH, alkyloxy; R2 = alkyl, aralkyl, Ph; R3 = alkyl, Ph, pyridyl, imidazolyl), useful as 17.alpha.-hydroxylase/C17-20-lyase inhibitors, thromboxane A2 synthesis inhibitors, and aromatase inhibitors, were prepd. I (R1 = H, R2 = Me, R3 = 3-pyridyl) showed 17.alpha.-hydroxylase/C17-20-lyase and aromatase inhibitor

157058-45-2P 157058-46-3P 157058-47-4P 221651-52-1P 221651-54-3P 221651-56-5P 221651-61-2P 221651-64-5P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of dihydronaphthalenes)

ANSWER 14 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

226571-57-9P

RL: RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of .alpha.2B and .alpha.2C adrenoceptor agonists)

226571-57-9 CAPLUS 1-Naphthalenol, 1,2,3,4-tetrahydro-2-(lH-imidazol-4-ylmethyl)-7-methoxy-(9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 15 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

(Continued)

157058-45-2 CAPLUS

1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-5-methoxy-(9CI) (CA INDEX NAME)

157058-46-3 CAPLUS

1(2H) -Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-6-methoxy-(9CI) (CA INDEX NAME)

157058-47-4 CAPLUS 1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-7-methoxy-(9CI) (CA INDEX NAME)

221651-52-1 CAPLUS 1(2H)-Naphthalenone, 5-ethoxy-3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-CN (9CI) (CA INDEX NAME)

221651-54-3 CAPLUS 1(2H)-Naphthalenone, 6-ethoxy-3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-(9CI) (CA INDEX NAME)

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ANSWER 15 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

221651-56-5 CAPLUS RN

1(2H)-Naphthalenone, 7-ethoxy-3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-(9CI) (CA INDEX NAME)

221651-61-2 CAPLUS

1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-6-propoxy-(9CI) (CA INDEX NAME)

221651-64-5 CAPLUS

1(2H)-Naphthalenone, 3,4-dihydro-2-(lH-imidazol-4-ylmethyl)-6-(2methylpropoxy) - (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 16 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) study, unclassified); PRP (Properties); RCT (Reactant); SFN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (synthesis and evaluation of azole-substituted tetrahydronaphthalenes as inhibitors of human and lab. animal cytochrome P 450 enzymes in relation to structure and hormone formation and uterotropic activity

and mammary tumor inhibition) 157058-44-1 CAPLUS

1(2H) -Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl) - (9CI) (CA

1(2H) -Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-5-methoxy-(9CI) (CA INDEX NAME)

157058-46-3 CAPLUS ĆN 1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-6-methoxy-(9CI) (CA INDEX NAME)

157058-47-4 CAPLUS 1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-7-methoxy-(9CI) (CA INDEX NAME)

157058-52-1P 157058-53-2P 157058-55-4P 178880-06-3P

L6 ANSWER 16 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:358249 CAPLUS

DOCUMENT NUMBER: 125:75343

Synthesis and evaluation of azole-substituted TITLE: tetrahydronaphthalenes as inhibitors of P450 arom,

P450 17 and P450 TxA2 AUTHOR(S):

Hartmann, Rolf W.; Frotscher, Martin; Ledergerber, Dorothea; Waechter, Gerald A.; Gruen, Gertrud L.;

Sergejew, Tom F.

Fachrichtung 12.1 Pharmazeutische Chemie, Univ. Saarlandes, Saarbruecken, D-66041, Germany CORPORATE SOURCE: SOURCE:

Archiv der Pharmazie (Weinheim, Germany) (1996),

329(5), 251-261

CODEN: ARPMAS: ISSN: 0365-6233

PUBLISHER: VCH DOCUMENT TYPE: Journal

LANGUAGE:

UAGE: English
In search of potential drugs for the treatment of estrogen- and androgen-dependent cancer as well as the prophylaxis of metastases, tetralones, tetralins, and dihydronaphthalenes bearing of OCH3 substituent at the benzene nucleus and an imidazol-4-yl, imidazol-1-yl, or 1,2,4-triazol-1-yl substituents in 2-position were synthesized with and without C2-spacer between the rings. The compds. were tested in vitro for inhibition of the three target enzymes P 450 arom (human placental microsomes), P 450 17 (rat testicular microsomes), and P 450 TxA2 (citrated human whole blood). To examine selectivity, some compds. were further tested in vitro for inhibition of P 450 18 (bovine adrenal mitochondrial), P 450 scc (bovine adrenal mitochondrial) and corticoid formation (aldosterone, corticosterone; ACTH stimulated rat adrenal tissue). In vivo, selected compds. were examd. in Sprague Dawley rats regarding P 450 TxA2 inhibition, redn. of plasma testosterone concn., antiuterotropic activity (inhibition of the uterotropic activity of androstenedione), redn. of plasma estradiol concn. (pregnant mares' serum gonadotropin-primed rats), and mammary tumor inhibiting activity (dimethylbenzanthracene-induced tumor; pre- and postmenopausal model). In the series of imidazol-4-yl compds., which represent new azole inhibitors of steroidogenic P 450 enzymes, strong inhibitors of P 450 arom and/or P 450 17 were found: 7-OCH3-2-(imidazol-4-ylmethylene)-1-tetralone (I) and 7-OCH3-2-(imidazol-4-ylmethyl)-tetralin (II) are among the most potent inhibitors of P 450 arom in vitro know so far. I is a selective inhibitor, whereas II shows in addn. strong inhibition of P 450 17. In contrast to II, the 6-OCH3 deriv. is a selective inhibitor of P 450 17, being 50 times more potent than ketoconazole. Some imidazol-1-ył compds. show a marked inhibition of P 450 TxA2: 2-(imidazol-1-ylmethyl)-1tetralone is a selective inhibitor of P 450 TxA2, whereas 7-0CH3-2-(imidazol-1-ylmethyl)-tetralin as well as 2-(imidazol-1-ylmethyl)tetralin and 7-OCH3-2-imidazol-1-yl-3,4-dihydronaphthalene addnl. show strong inhibition of P 450 arom and P 450 17. Structure-activity relations are discussed. Regarding the other steroidogenic P 450 enzymes as well as corticosterone formation, the compds. show only slight inhibitory activity. Aldosterone formation, however, is inhibited at low concns. Nevertheless, I and II are more selective, i.e. inhibit aldosterone synthesis less than the well known inhibitor of P 450 arom fadrozole. The compds. show activity in the aforementioned in vivo tests. 157058-44-1P 157058-45-2P 157058-46-3P

157058-47-4P RL: BAC (Biological activity or effector, except adverse); BSU (Biological

ANSWER 16 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(synthesis and evaluation of azole-substituted tetrahydronaphthalenes as inhibitors of human and lab. animal cytochrome P 450 enzymes in relation to structure and hormone formation and uterotropic activity and mammary tumor inhibition)

157058-52-1 CAPLUS

 $1 \\ H-Imidazole, \ 4-[(1,2,3,4-tetrahydro-2-naphthalenyl)methyl] + \ (9CI) \ (CA)$ INDEX NAME)

1H-Imidazole, 4-[(1,2,3,4-tetrahydro-5-methoxy-2-naphthalenyl)methyl]-(9CI) (CA INDEX NAME)

157058-55-4 CAPLUS

1H-Imidazole, 4-[(1,2,3,4-tetrahydro-7-methoxy-2-naphthalenyl)methyl]-CN (9CI) (CA INDEX NAME)

$$\mathsf{MeO} = \mathsf{CH}_2 = \mathsf{H}_{\mathsf{N}}$$

178880-06-3 CAPLUS

1H-Imidazole, 4-{(1,2,3,4-tetrahydro-6-methoxy-2-naphthalenyl)methyl}-,

ethanedioate (1:1) (9CI) (CA INDEX NAME)

CRN 157058-54-3 CMF C15 H18 N2 Q

Page 38 01/13/2004

ANSWER 16 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

CM 2

CRN 144-62-7 CMF C2 H2 O4

L6 ANSWER 18 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1995:827732 CAPLUS

DOCUMENT NUMBER:

AUTHOR(S):

124:202093

TITLE:

Molecular design of novel PGI2 agonists without PG skeleton. IV. [Erratum to document cited in

CA123:198689]

Hamanaka, N.; Takahashi, K.; Nagao, Y.; Torisu, K.;

Tokumeto, H.; Kondo, K. CORPORATE SOURCE: Minase Res. Inst., Ono Pharmaceutical Co., Ltd.,

Osaka, 618, Japan

SOURCE: Bioorganic & Medicinal Chemistry Letters (1995),

5(18), 2179

CODEN: BMCLE8; ISSN: 0960-894X PUBLISHER: Elsevier

DOCUMENT TYPE: Journal LANGUAGE: English

The errors were not reflected in the abstr. or the index entries.

150559-29-8 RL: BAC (Biological activity or effector, except adverse); BSU (Biological > study, unclassified); BIOL (Biological study) (PGI2 agonist activity of (Erratum))

150559-29-8 CAPLUS

Acetic acid, [[6-[[2-(diphenylmethyl)-lH-imidazol-4-yl]methyl]-5,6,7,8tetrahydro-1-naphthalenyl]oxy]- (9CI) (CA INDEX NAME)

L6 ANSWER 17 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1996:97011 CAPLUS

ACCESSION NUMBER:

124:260928 DOCUMENT NUMBER:

Novel nonprostanoid prostacyclin (PGI2) mimetics with TITLE:

heterocyclic moiety Nagao, Yuuki; Takahashi, Kanji; Torisu, Kazuhiko; AUTHOR (S):

Kondo, Kigen; Hamanaka, Nobuyuki Minase Res. Inst., Ono Pharmaceutical Co., Ltd., Osaka, 618, Japan CORPORATE SOURCE:

Heterocycles (1996), 42(2), 517-23 SOURCE: CODEN: HTCYAM; ISSN: 0385-5414

PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal LANGUAGE:

Structural modification of [[6-[2-[(diphenylmethoxy)imino]pentyl]-5,6,7,8-tetrahydro-1-naphthalenyl]oxy]acetic acid [i.e., [2-(2-benzhydryloxyiminopentyl)-1,2,3,4-tetrahydro-5-naphthyloxy]acetic acid], previously identified as a PGI2 agonist without a PG skeleton, was exame.

Such analogs were for example, [[6-[[3-(diphenylmethyl)-1,2,4-oxadiazol-5-y]]methyl]-5,6,7,8-tetrahydro-1-naphthalenyl]oxy]acetic acid or [[6-[[2-(diphenylmethyl)-1H-imidazol-4-yl]methyl]-5,6,7,8-tetrahydro-1-naphthalenyl]oxy]acetic acid. Conversion of the oxime moiety in [[6-[2-[(diphenylmethoxy)imino]pentyl]-5,6,7,8-tetrahydro-1-naphthalenyl]oxy]acetic acid.

naphthalenyl]oxy]acetic acid to a pyrazole led to [[6-[[4-(diphenylmethyl)-1H-pyrazol-l-yl]methyl]-5,6,7,8-tetrahydro-1-naphthalenyl]oxy]acetic acid [i.e., [2-(4-benzhydrylpylazoyl)methyl-1,2,3,4-tetrahydro-5-

naphthyloxy]acetic acid] which strongly inhibited ADP-induced aggregation of human platelets in vitro.

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of [{[[(phenylmethoxy)imino}alkyl]naphthalenyl]oxy]acetate

analogs as nonprostancid prostacyclin mimetics)
150559-29-8 CAPLUS
Acetic acid, [[6-[[2-(diphenylmethyl)-1H-imidazol-4-yl]methyl]-5,6,7,8-tetrahydro-1-naphthalenyl]oxy]- (9CI) (CA INDEX NAME)

HO2C-CH2-0

L6 ANSWER 19 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:612212 CAPLUS

DOCUMENT NUMBER: 123:198691

Medetomidine analogs as .alpha.-adrenergic agonists Amemiya, Yoshiya; Hus, Fulian; Shams, Gamal; Feller, Dennis R.; Venkataraman, B. V.; Patil, Popat N.; TITLE: AUTHOR(S):

CORPORATE SOURCE: College Pharmacy, Ohio State University, Columbus, OH,

43210, USA

Egyptian Journal of Pharmaceutical Sciences (1994), 35(1-6), 403-10 SOURCE:

CODEN: EJPSBZ: ISSN: 0301-5068

National Information and Documentation Centre PUBLISHER:

DOCUMENT TYPE: LANGUAGE: English

OTHER SOURCE(S): CASREACT 123:198691

Recently, it has been reported that medetomidine is a new 4-substituted imidazole analog possessing selective and potent .alpha.2-adrenergic properties. It has been shown that it reduces blood pressure, heart rate and saliva secretion. At the present time is sedative and hypotensive effects seem to be manifest in the same dose range. We have initiated a program to see if it is possible to sep. these activities with analogs of medetomidine. The initial studies have been directed at procedures for the conversion of the imidazolines, a common structure of .alpha.-adrenergic drugs, to the corresponding imidazoles. It was found that 2-substituted and 2,4-disubstituted imidazolines can easily

converted into imidazoles using 10% Pd/C in refluxing toluene, while in some instances there are some difficulties with the conversion of 4-substituted imidazolines to the imidazoles. The synthesis of 1- or 2-(2-or 4-imidazolylmethyl)naphthalene analogs of medetomidine are also 137967-88-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); BIOL (Biological study): PREP (Preparation)

(prepn. of 4-substituted imidazoles)

137967-88-5 CAPLUS 1H-Imidazole, 4-[1-(2-naphthalenyl)ethyl]- (9CI) (CA INDEX NAME)

Page 39 01/13/2004

ANSWER 20 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:612188 CAPLUS

123:111932 DOCUMENT NUMBER:

Synthesis and .alpha.-adrenergic activities of 2- and TITLE: 4-substituted imidazoline and imidazole analogs of

.alpha.- and .beta.-naphthalene Amemiya, Yoshiya; Venkataraman, Burrah V.; Patil,

AUTHOR (S): Popat N.; Shams, Gamal: Romstedt, Karl

College Fharmacy, Ohio State University, Columbus, OH, CORPORATE SOURCE:

43210, USA Egyptian Journal of Pharmaceutical Sciences (1994), 35(1-6), 91-112

CODEN: EJPSBZ; ISSN: 0301-5068

National Information and Documentation Centre PUBLISHER:

DOCUMENT TYPE: Journal LANGUAGE: English

SOURCE:

Seven analogs of medetomidine and naphazoline were synthesized and evaluated for their .alpha.1- (aorta) and .alpha.2- (platelet) activities. The analogs were composed of 2- and 4-substituted imidazoles and imidazolines attached through a methylene bridge to either an alpha. - or .beta. -naphthalene ring system. In general the .alpha. -naphthlene analogs were found to be the most potent inhibitors of platelet aggregation. .alpha. -Naphthalene analogs were partial agonists while the .beta.-naphthalene analogs were antagonists in .alpha.1-adrenergic system

(aorta). 137967-82-9P 166034-65-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and adrenergic activities of medetomidine and naphazoline analogs)

137967-82-9 CAPLUS

1H-Imidazole, 4-[1-(2-naphthalenyl)ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

HC1

166034-65-7 CAPLUS

1H-Imidazole, 4-[1-(2-naphthalenyl)ethyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 137967-88-5 CMF C15 H14 N2

L6 ANSWER 21 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1995:598392 CAPLUS DOCUMENT NUMBER: 123:198689

Molecular design of novel PGI2 agonists without PG TITLE:

skeleton. IV AUTHOR (S):

Hamanaka, Nobuyuki; Takahasi, Kanji; Nagao, Yuuki; Torisu, Kazuhiko; Tokumoto, Hidekado; Kondo, Kigen CORPORATE SOURCE: Minase Res. Inst., One Pharmaceutical Co., Ltd.,

Osaka, 618, Japan

Bioorganic & Medicinal Chemistry Letters (1995), SOURCE:

5(10), 1083-6

CODEN: BMCLE8; ISSN: 0960-894X PUBLISHER:

Elsevier DOCUMENT TYPE: Journal

English

LANGUAGE:

OCH2CO2H

The synthesis and biol. evaluation of a novel series of di- or tetrahydronaphthalen-5-oxyacetic acid derivs. with a 4-benzhydrylpyrazolyl group is described. Among these compds., I has been identified as a highly potent PGI2 agonist with an exceptionally long in vivo duration of

150559-29-8 ΙT

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(PGI2 agonist activity of) 150559-29-8 CAPLUS

Acetic acid, [[6-[[2-(diphenylmethyl)-lH-imidazol-4-yl]methyl]-5,6,7,8-

tetrahydro-1-naphthalenyl]oxy]- (9CI) (CA INDEX NAME)

$$CH_2$$
 CH_2
 N
 $CHP h_2$
 N
 N

ANSWER 20 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

CM 2

CRN 144-62-7 CMF C2 H2 O4

137967-88-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and adrenergic activities of medetomidine and naphazoline

137967-88-5 CAPLUS

1H-Imidazole, 4-[1-(2-naphthalenyl)ethyl]- (9CI) (CA INDEX NAME)

L6 ANSWER 22 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN 1995:513524 CAPLUS

ACCESSION NUMBER:

DOCUMENT NUMBER: 122:265379 TITLE:

Preparation of (cyanobenzyl) azole derivatives as aromatase inhibitors

INVENTOR(S): Shibata, Tomoyuki; Sugimura, Yukio; Tanzawa, Kazuhiko; Takahashi, Masaaki: Kobayashi, Tomowo: Mitsuhashi,

Yoshihiro PATENT ASSIGNEE(S):

Sankyo Co., Ltd., Japan PCT Int. Appl., 94 pp. CODEN: PIXXD2

Patent

DOCUMENT TYPE: LANGUAGE:

SOURCE:

Japanese

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE WO 9408973 A1 19940428 WO 1993-JP1509 19931020 W: AU, CA, CZ, FI, HU, KR, NO, NZ, RU, US RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE AU 9352855 A1 19940509 AU 1993-52855 19931020 19940509 JP 06263742 JP 1993-261438 19931020 19940920 A2 PRIORITY APPLN. INFO.: JP 1992-283177 19921021 WO 1993-JP1509 19931020

The title compds. (I; R1 = imidazolyl, triazolyl or tetrazolyl each of which may be substituted by Me and/or Et; R2 = naphthyl, phenanthryl or anthryl each of which may be substituted by substituent(s) selected from C1-4 alkyl, C1-4 alkoxy, C1-6 acyloxy, arom. acyloxy, OH, trialkyl, C1-4 acylamino, alkoxyalkoxy, alkoxyacyloxy, and trialkylsilyloxy, R3 = H, Me, cyano), useful for the treatment of breast cancer, are prepd. Thus, 2-bromo-6-methoxynaphthalene was treated with BuLi in hexane and THF at

Page 40 01/13/2004

L6 ANSWER 22 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN -78.degree. followed reaction with a soln. of p-cyanobenzaldehyde in THF at -78.degree. gave p-cyano-.alpha.-(6-methoxynaphthalen-2-yl)benzyl alc. which was stirred with SOC12 in CH2C12 at room temp. for 1 h to give p-cyano-.alpha.-(6-methoxynaphthalen-2-yl)benzyl chloride. The latter chloride was dissolved in MeCN and refluxed with imidazole overnight to give, after silica gel chromatog, and acidification with HCl, title compd. (II.HCl) which in vitro showed IC50 of 3.7 nM against aromatase. Hard capsule, tablet, injection and suspension formulations contg. (p-cyanobenzyl) tetrazole deriv. (III.HCl) were described.

162573-42-4P 162573-46-8P 162573-58-2P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of (cyanobenzyl) azole deriv. as aromatase inhibitor and anticancer agent for breast cancer) 162573-42-4 CAPLUS

Benzonitrile, 4-(lH-imidazol-4-yl-2-naphthalenylmethyl)- (9CI) (CA INDEX

162573-46-8 CAPLUS Benzonitrile, 4-(lH-imidazol-4-yl-9-phenanthrenylmethyl)- (9CI) (CA INDEX

162573-58-2 CAPLUS Benzonitrile, 4-(1H-imidazol-4-yl-2-naphthalenylmethyl)-,

monohydrochloride (9CI) (CA INDEX NAME)

L6 ANSWER 23 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1994:534112 CAPLUS

DOCUMENT NUMBER: 121:134112

Preparation of imidazolylmethylenetetralones and analogs as aromatase inhibitors

INVENTOR (S): Hartmann, Rolf W.; Wachter, Gerald Anton

PATENT ASSIGNEE(S): Tokyo Tanabe Co. Ltd., Japan SOURCE:

PCT Int. Appl., 29 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PA	PATENT NO.				KIND DATE					APPL	I CAT I	0.	DATE				
WO	9407	866		A.	1	1994	0414		1	WO 1	993-J	P143	3	1993	1006		
	W:	ΑU,	BB,	BG,	BR,	CA,	CZ,	FI,	HU	, KR	, LK,	MG,	MN,	MW,	NO,	NZ,	PL,
						UA,											
	RW:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB	, GR	IE,	ΙT,	LU,	MC,	NL,	PT,	SE,
		BF,	ВJ,	CF,	CG,	CI,	.CM,	GA,	GN	, ML	MR,	NE,	SN,	TD,	TG		
	9351											1184					
JP	0619	2233		A2	2	1994	0712			JP 15	993-2	5025	7	1993	1006		
PRIORITY	APP:	LN. 1	NFO.	:					JP	1992	-2671	30	Α	1992	1006		
								V	VO.	1993-	-JP14	33	W	1993	1006		
OTHER SO	URCE	(S):			MAR	PAT	121:	13411	12								

GΙ

The title compds. I [R represents hydrogen, C1-C4 lower alkoxy, nitro or C1-C4 lower alkoxycarbonyl; when X and Y represent each hydrogen or X and Y are combined together to represent oxygen, Z represents hydrogen and the broken line represents an arbitrary bond; when X represents hydrogen, Y and Z are combined together to represent a single bond, n represents an integer of 0 or 1] are prepd. A mixt. of 1-tetralone and imidazole-4-carbaldehyde in 40% H2SO4 was heated for 20 h at 80-90.degree. to give, after workup, (E)-2-(4-imidazolylmethylene)-1-tetralone (II). If in vitro showed IC50 of 0.260 .mu.M against aromatase.

157058-44-1P 157058-45-2P 157058-46-3P 157058-47-4P 157058-52-1P 157058-53-2P

157058-54-3P 157058-55-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of, as aromatase inhibitor) 157058-44-1 CAPLUS

1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)- (9CI) (CA

ANSWER 22 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

HCl

ANSWER 23 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

157058-45-2 CAPLUS RN 1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-5-methoxy-CN (9CI) (CA INDEX NAME)

157058-46-3 CAPLUS 1(2H)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-6-methoxy-

157058-47-4 CAPLUS CN 1(ZH)-Naphthalenone, 3,4-dihydro-2-(1H-imidazol-4-ylmethyl)-7-methoxy-(9CI) (CA INDEX NAME)

157058-52-1 CAPLUS CN 1H-Imidazole, 4-[(1,2,3,4-tetrahydro-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

157058-53-2 CAPLUS

1H-Imidazole, 4-[(1,2,3,4-tetrahydro-5-methoxy-2-naphthalenyl)methyl]-

Page 41 01/13/2004

ANSWER 23 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) (9CI) (CA INDEX NAME)

157058-54-3 CAPLUS $1 \\ H-Imidazole, \ \ 4-[(1,2,3,4-tetrahydro-6-methoxy-2-naphthalenyl) \\ methyl]-1 \\ T-1 \\ T-2 \\ T-2 \\ T-3 \\ T-4 \\ T-4$ (9CI) (CA INDEX NAME)

157058-55-4 CAPLUS 1H-Imidazole, 4-[(1,2,3,4-tetrahydro-7-methoxy-2-naphthalenyl)methyl]-(9CI) (CA INDEX NAME)

L6 ANSWER 24 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) но2с-сн2-о

150559-29-8 CAPLUS Acetic acid, [[6-[[2-(diphenylmethyl)-1H-imidazol-4-yl]methyl]-5,6,7,8tetrahydro-1-naphthalenyl] oxy] - (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2 \\ \text{HO}_2\text{C}-\text{CH}_2-\text{O} \end{array}$$

L6 ANSWER 24 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1993:671157 CAPLUS 119:271157 DOCUMENT NUMBER: TITLE: Fused benzeneoxyacetic acid derivative PGI2 receptor INVENTOR(S): Hamanaka, Nobuyuki; Takahashi, Kanji; Tokumoto, Hidekado PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan SOURCE: Eur. Pat. Appl., 110 pp. CODEN: EPXXDW DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE EP 548949 EP 1992-121898 19921223 A2 19930630 EP 548949 19931006 A3 EP 548949 19970917 В1 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE JP 05178832 A2 19930720 JP 1991-360502 19911227 JP 07025854 A2 19950127 JP 1992-209587 19920714 19951024 US 1992-912999 CA 1992-2073917 US 5461045 A AA 19920714 CA 2073917 19940116 19920715 CA 2085844 CA 1992-2085844 19930628 AA 19921218 AT 158282 19971015 AT 1992-121898 19921223 ES 2108076 Т3 19971216 ES 1992-121898 19921223 US 5389666 19950214 US 1992-997492 19921228 JP 07145057 19950606 20030623 A2 JP 1992-360608 19921228 JP 3419009 B2 US 5589496 19961231 US 1994-334395 19941103 Α US 5849919 19981215 US 1996-722456 19960927 US 5962439 19991005 US 1998-168424 19981007 PRIORITY APPLN. INFO.; JP 1991-360502 19911227 JP 1992-209587 19920714 US 1992-997492 A3 19921228 US 1994-334395 A3 19941103 US 1996-722456 A3 19960927 OTHER SOURCE(S): MARPAT 119:271157 For diagram(s), see printed CA Issue. The title compds. I [A = (un)substituted heterocyclyl; B = alkylene, alkenylene; ring D = carbocyclic ring; R1 = HO, C1-12 alkoxy, (un)substituted amino], which demonstrate PGI2 receptor agonist activity and are useful in the treatment of thrombosis, arteriosclerosis, ischemic heart diseases, gastric ulcer, or hypertension (no data), are prepd. and I-contg. formulations presented. Thus, pyrazole deriv. II was prepd. which demonstrated 50% inhibitory concn. against human blood platelet aggregation of 0.043 .mu.M in human blood-derived. platelet-rich plasma. 150558-87-5 150559-29-8 RL: RCT (Reactant); RACT (Reactant or reagent) (PGI2 receptor agonist activity of)

L6 ANSWER 25 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1993:649949 CAPLUS DOCUMENT NUMBER: 119:249949 TITLE: Preparation of imidazole derivatives as interleukin 1 inhibitors and antiphlogistics INVENTOR (5): Veno, Yoshihide; Masumori, Hiroaki; Saji, Kitaro

Acetic acid, [[5,6,7,8-tetrahydro-6-(lH-imidazol-4-ylmethyl)-1-naphthalenyl]oxy]- (9CI) (CA INDEX NAME)

PATENT ASSIGNEE(S): Sumitomo Pharma, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp. CODEN: JKXXAF

DOCUMENT TYPE: LANGUAGE: Japanese FAMILY ACC. NUM. COUNT:

PATENT INFORMATION: PATENT NO. KIND DATE

150558-87-5 CAPLUS

JP 05155882 A2 19930622 JP 1991-348294 19911203 PRIORITY APPLN. INFO.: JP 1991-348294 19911203 OTHER SOURCE(S): MARPAT 119:249949 For diagram(s), see printed CA Issue.

The title derivs. I {A = lower alkylene; M = arom. hydrocarbon ring,

thiophene: D = 0, CO, CH(CR5), C(:NOR5), CH[N(R5)2], NR5, single bond: R1H, halo; R2 = lower alkyl or alkenyl, (un) substituted Ph, (un) substituted cycloalkyl, (un) substituted thienyl; R3 = N-contg. heterocyclyl; R4, R5 = H, lower alkyl; when D is single bond then R2 is lower alkokyl or their acid salts are prepd. as interleukin 1 inhibitors and antiphlogistics. A mixt. of 3-(2-fluoro-4-biphenyl)-1-(4pyridylcarbonyl)amino-2-butanone (prepd. from fluorobiprofen in 4 steps), and NH4Ac was heated at 140-150.degree. for 4 h to give 44% 4-(1-(2-fluoro-4-biphenyl)ethyl)-2-(4-pyridyl)imidazole-HCl. I inhibited growth of interleukin 1.

APPLICATION NO. DATE

150972-40-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, as interleukin 1 inhibitor and antiphlogistics) 150972-40-0 CAPLUS

2-Naphthalenol, 6-[1-[2-(4-pyridinyl)-lH-imidazol-4-yl]ethyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Page 42 01/13/2004

L6 ANSWER 26 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:106173 CAPLUS DOCUMENT NUMBER: 116:106173

Synthesis and .alpha.-adrenergic activities of 2- and 4-substituted imidazoline and imidazole analogs AUTHOR (S):

Amemiya, Yoshiya; Hong, Seoung S.; Venkataraman, Burrah V.; Patil, Popat N.; Shams, Gamal; Romstedt, Karl; Feller, Dennis R.; Hsu, Fu Lian; Miller, Duane

CORPORATE SOURCE: Coll. Pharm., Ohio State Univ., Columbus, OH, 43210,

Journal of Medicinal Chemistry (1992), 35(4), 750-5 SQURCE: CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal English

LANGUAGE:

Analogs I-III (R = 1-naphthyl, 2-naphthyl; R1 = H, Me) of medetomidine and naphazoline were synthesized and evaluated for their .alpha.l (aorta) and alpha.2 (platelet) activities. In general the 1-naphthalene analogs were the most potent inhibitors of epinephrine-induced platelet aggregation. Of considerable interest was the fact that I-III (R = 1-naphthyl) were antagonists in an .alpha.1-adrenergic system (aorta). Thus, appropriately substituted naphthalene analogs of medetomidine and naphazoline provide a spectrum of .alpha.l-agonist, .alpha.l-antagonist, and .alpha.2-antagonist

activity. 137967-82-9P 137967-88-5P

RL: SPN (Synthetic preparation): PREP (Preparation)

(prepn. and adrenergic activity of)

137967-82-9 CAPLUS

1H-Imidazole, 4-[1-(2-naphthalenyl)ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

137967-88-5 CAPLUS

1H-Imidazole, 4-[1-(2-naphthalenyl)ethyl]- (9CI) (CA INDEX NAME)

L6 ANSWER 27 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN 1992:15364 CAPLUS

ACCESSION NUMBER:

DOCUMENT NUMBER: 116:15364 TITLE:

Structure-activity studies of new imidazolines on adrenoceptors of rat aorta and human platelets Venkataraman, B. V.; Shams, G.; Hamada, A.; Amemiya, AUTHOR(S):

Y.; Tantishaiyakul, V.; Hsu, F.; Fashempour, J.;

Romstedt, K. J.; Miller, D. D.; et al.

CORPORATE SOURCE: Coll. Pharm., Ohio State Univ., Columbus, OH, 43210,

USA SOURCE:

Naunyn-Schmiedeberg's Archives of Pharmacology (1991), 344(4), 454-63 CODEN: NSAPCC; ISSN: 0028-1298

DOCUMENT TYPE: Journal

LANGUAGE: English

Potencies of new arom, substituted fluoro or iodo analogs of catecholimidazoline (I) on functional responses in rat aorta (.alpha.1) and platelets (.alpha.2) were quantified. When compared either on the basis of EC50 or the dissoon. const. (KA), 5-fluorocatecholimidazoline was as potent as the ref. .alpha.l-adrenoceptor agonist, phenylephrine in the vascular tissue. The max. contraction of aorta produced by the fluoro analog was, however, 17% higher than that of phenylephrine. The time required for 1/2 relaxation of the tissue after 5-fluoro hydroxy imidazoline was at least twice as long as that of the phenylephrine. The catechol moiety as well as fluorine substitution at the crit. 5-position of the arom. ring is essential for higher .alpha.1 adrenoceptor-mediated potency. As compared to the fluoro analogs, the adrenoceptor-mediated potencies of iodo-analogs were relatively weak on vascular tissue. Naphazoline and its analogs were partial agonists on vascular tissue with dissocn. consts, which ranged from 110 to 2600 nmol/L. Imidazole analogs (II, R = naphthyl or xylene), were generally less potent agonist than the imidazolines by one order of magnitude. The vascular effects of all agonists were competitively blocked by prazosin with KB values which ranged from 0.04 to 0.48 nmol/L. Since the variation in KB values were within normal limits, the action of new imidazolines on rat aorta appears to be mediated mainly by the activation of the .alpha.1-adrenoceptor. Prazosin 10 nmol/L abolished the vascular response of some partial agonists. This indicates a slightly different mode of interaction of agonists with the transduction process. Carbon 4-substituted imidazolines produced little or no .alpha.1 adrenoceptor-mediated intrinsic activity, but competitive receptor blocking potency was comparable to that of phentolamine. Medetomidine was a partial agonist on the rat aorta with a KA of 260 mol/L. When investigated as a blocker, the KB of medetomidine against phenylephrine was approx. 5600 nmol/L. The variation in the latter value was high. In acetylsalicylic acid-treated human platelets, the .alpha.2-adrenoceptor-mediated aggregatory effect of all fluoro analogs was weak. Iodo or naphazoline analogs did not initiate platelet

ANSWER 26 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

- L6 ANSWER 27 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN aggregation but blocked the aggregation induced by epinephrine. The affinity of naphazoline for the .alpha.2-adrenoceptor was 1100 nmol/L. The IC50 of medetomidine for platelet anti-aggregatory effect was 3300 nmol/L, which compares favorably with other imidazoline type of blockers of platelet aggregations. Sympathomimetic vasoconstrictor actions and platelet aggregation effects of these compds. can be dissocd. Some vasoconstrictors were antiaggregatory. The structure-activity relationships of the two receptor systems, namely rat aorta (.alpha.l) and platelets (.alpha.2), are discussed.
- 137967-88-5

RL: BIOL (Biological study)

(.alpha.-adrenoceptors of aorta and human platelets interaction with,

structure in relation to) 137967-88-5 CAPLUS

1H-Imidazole, 4-[1-(2-naphthalenyl)ethyl]- (9CI) (CA INDEX NAME)

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L6 ANSWER 28 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1991:623482 CAPLUS 115:223482 DOCUMENT NUMBER: Use of 5-HT3 receptor antagonists for treatment of TITLE: panic disorders, agoraphobia, or obsessive compulsive disorders Azcona, Alberto INVENTOR (5): Sandoz-Erfindungen Verwaltungsgesellschaft m.b.H., PATENT ASSIGNEE(S): Austria: Sandoz-Patent-G.m.b.H.: Sandoz A.-G. PCT Int. Appl., 35 pp. SOURCE: CODEN: PIXXD2 DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: PATENT INFORMATION: APPLICATION NO. DATE PATENT NO. KIND DATE wo 9012569 A1 19901101 WO 1990-EP540 19900406 W: AU, CA, JP, KR, US RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE 2031214 AA 19901022 CA 1990-2031214 19900406 19901022 19901116 CA 2031214 AU 9054158 AU 1990-54158 19900406 **A**1 19921203 AU 631632 19910417 EP 1990-905482 19900406 EP 422154 EP 422154 В1 19931201 R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE 03505881 T2 19911219 JP 1990-505770 19900406 JP 03505881 B4 19940907 JP 06069963 AT 1990-905482 AT 97803 19931215 19900406 ES 1990-905482 19900406 ES 2061024 **T**3 19941201 ZA 1990-3015 US 1994-187413 19900420 ZA 9003015 19911224 19940124 HS 5530008 Α 19960625 PRIORITY APPLN. INFO.: 19890421 GB 1989-9147 GB 1989-16602 19890720 EP 1990-905482 19900406 WO 1990-EP540 19900406 US 1990-635156 19901219 5-HT3 receptor antagonists are useful in treating panic disorders and/or agoraphobia or obsessive compulsive disorders. Formulations for tablets, AΒ i.v. solms. and capsules are presented. 135716-73-3 RL: BIOL (Biological study) (5-HT3 receptor antagonist) 135716-73-3 CAPLUS 1(2H)-Phenanthrenone, 3,4-dihydro-2-[(5-methyl-1H-imidazol-4-yl)methyl]-(9CI) (CA INDEX NAME)

ANSWER 29 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: DOCUMENT NUMBER:

1990:198377 CAPLUS 112:198377

Preparation and formulation of imidazole derivatives

TITLE:

as 5-HT3 receptor antagonists North, Peter Charles: Oxford, Alexander William;

INVENTOR(S):

Coates, Ian Harold Glaxo Group Ltd., UK

PATENT ASSIGNEE(S): SOURCE:

Eur. Pat. Appl., 12 pp. CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
		-		
EP 336759	A1	19891011	EP 1989-303415	19890406
R: AT, BE,	CH, DE	ES, FR, G	B, GR, IT, LI, LU, NL	, SE
JP 02049772	A2	19900220	JP 1989-87841	19890406
US 5116984	A	19920526	US 1989-333967	19890406
PRIORITY APPLN. INFO.	. :		GB 1988-8085	19880407
			GB 1988-8086	19890407
OTHER SOURCE(S):	MA	RPAT 112:19	8377	

(cH₂) n

Title compds. I (R1, R2 = H, halo, H0, C1-4 alkoxy, C1-4 alkyl, C1-4 alkylthio, R3R4N, R3, R4 = H, C1-4 alkyl, R3R4N = satd. 5-7-membered ring; A = CH, N: Im = substituted imidazolyl: n = 1-3) and physical. acceptable salts and solvates thereof, potent and selective antagonists of 5-HT3 receptors and useful, e.g., in treatment of psychotic disorders, anxiety, and nausea and vomiting (no data), are prepd. 1,2-Dihydro-3-[[5-methyl-1-(triphenylmethyl)-IH-imidazol-4-yl]methylene]-4(3H)-phenanthrenone (prepn block) and daydrogneted solver BdC to give I (Bl. 82 m H) A = CH. Im m given) was dehydrogenated over Pd/C to give I (RI, R2 = H; A = CH; Im = 5-methylimidazol-4-yl; n = 2) which was converted to the maleate. Tablet and injection formulations were given.

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, as 5-HT antagonist) 126737-68-6 CAPLUS

4(1H)-Phenanthrenone, 2,3-dihydro-3-((5-methyl-1H-imidazol-4-yl)methyl]-, CN (2Z)-2-butenedicate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 126737-65-3 CMF C19 H18 N2 O L6 ANSWER 28 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

ANSWER 29 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

(Continued)

CM 2

CRN 110-16-7 CMF C4 H4 04

Double bond geometry as shown.

H02C 2 CO2H

IT 126737-65-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, as HT3-receptor antagonist) 126737-65-3 CAPLUS

4(1H)-Phenanthrenone, 2,3-dihydro-3-[(5-methyl-1H-imidazol-4-yl)methyl]-(9CI) (CA INDEX NAME)

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ANSWER 30 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:139033 CAPLUS

DOCUMENT NUMBER: 112:139033

Preparation of imidazole derivatives as drugs Kihara, Noriaki; Tomino, Ikuo; Tan, Hiroaki; Takei, TITLE: INVENTOR(S): Mitsusachi

PATENT ASSIGNEE(S): Mitsui Petrochemical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF DOCUMENT TYPE: Patent

Japanese LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

APPLICATION NO. DATE PATENT NO. KIND DATE JP 01242571 A2 19890927 JP 1988-65731 19880322 JP 1988-65731 PRIORITY APPLN. INFO.: 19880322 MARPAT 112:139033

OTHER SOURCE(S):

$$R^{1}$$
 R^{1}
 R^{2}
 R^{3}
 R^{1}
 R^{2}
 R^{2}
 R^{2}
 R^{2}
 R^{3}
 R^{2}
 R^{2}
 R^{3}
 R^{2}
 R^{3}
 R^{2}
 R^{3}
 R^{4}
 R^{5}
 R^{7}

The title derivs. I or II (R1 = H, Ph; R2-R5 = H, OH, lower alkyl, lower alkoxy, lower alkylamino, halo; R2-R5 may be bonded to from rings; R6, R7 = H, lower alkyl, halo; X = O, S), useful as cerebral function improvers, antihypertensives, diuretics, etc. (no data), are prepd. by acid-catalyzed reaction of (hydroxymethyl)imidazoles III or their acid salts with benzenes IV or 5-membered heterocycle V. Thus, aq. III.HCl (Rl = H) was treated with 1,3,5-C6H3Me3 and 4-MeC6H4SO3H at 170.degree. for 7 h to give 768 I (Rl = R2 = H, R3-R5 = 2,4,6-Me3). 125883-69-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of, as drug) 125883-69-4 CAPLUS

1H-Imidazole, 4-(2-naphthalenylmethyl) - (9CI) (CA INDEX NAME)

L6 ANSWER 31 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1979:168771 CAPLUS

DOCUMENT NUMBER: 90:168771

Photochemical reactions. Photochemistry of N-acylimidazoles. V. Photolysis of the N-acylimidazoles of dehydroabietic acid and of TITLE: 13-deisopropyl-10-epi-dehydroabietic acid

AUTHOR(S): Iwasaki, Shigeo CORPORATE SOURCE:

Org.-Chem. Lab., ETH, Zurich, Switz. SOURCE:

Helvetica Chimica Acta (1978), 61(8), 2843-50 CODEN: HCACAV; ISSN: 0018-019X

DOCUMENT TYPE: English

LANGUAGE: GΙ

> CHMe 2 CHMe 2 М́е

Irradn. of I gave no Type II elimination, but gave II and III by migration of the imidazolylcarbonyl group, probably via a cyclobutanol intermediate. Similarly, irradn. of IV gave only a small amt. of Type II fragmentation, the main products being derived from .gamma.-H abstraction.

H

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of) 69634-29-3 CAPLUS RN

Methanone, lH-imidazol-4-yl[4b, 5, 6, 7, 8, 8a, 9, 10-octahydro-4b, 8-dimethyl-2-

(1-methylethyl)-9-phenanthrenyl]- (9CI) (CA INDEX NAME)

ANSWER 30 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

ANSWER 31 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN

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L6 ANSWER 32 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1973:515495 CAPLUS DOCUMENT NUMBER: 79:115495 TITLE: Synthesis of small molecule catalysts. Model for the active site of ribonuclease-A Algieri, Aldo A.
Cornell Univ., Ithaca, NY, USA
(1973) 116 pp. Avail.: Univ. Microfilms, Ann Arbor,
Mich., Order No. 73-14,715 AUTHOR(S):
CORPORATE SOURCE:
SOURCE: From: Diss. Abstr. Int. B 1973, 33(12)(Pt. 1), 5722 DOCUMENT TYPE: Dissertation LANGUAGE: English Unavailable AB 49738-45-6 RL: RCT (Reactant); RACT (Reactant or reagent) (as model for the active site of ribonuclease A) 49738-45-6 CAPLUS IH-Imidazole 4-ethanamine, N-{[3-(1H-imidazol-4-ylmethyl)-1naphthalenyl]methyl]-, conjugate diacid {9CI} (CA INDEX NAME)

●2 H+

L6 ANSWER 33 OF 33 CAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1972:501463 CAPLUS DOCUMENT NUMBER: 77:101463 Voges-Proskauer reaction. II. Structure of a pigment from the diacetyl reaction of 1-benzyl-1methylguanidine^{*} AUTHOR (S): Nishimura, Tamio; Yamazaki, Chiji; Ueno, Tetsuro; Kitajima, Shinichi; Ishige, Koichi Sch. Hyg. Sci., Kitasato Univ., Tokyo, Japan Bulletin of the Chemical Society of Japan (1972), CORPORATE SOURCE: SOURCE: 45(6), 1782-5 CODEN: BCSJA8; ISSN: 0009-2673 DOCUMENT TYPE: Journal LANGUAGE: English

A pigment formed by the reaction of 1-benzyl-1-methylguanidine was isolated as reddish purple prisms. The reduced pigment was colorless and rapidly converted back to the original pigment on exposure to the air. On the basis of ir, NMR, and mass spectral evidence, the structures of the pigment and the reduced form were established to be 2-(N-benzyl-N-thylgisto). $\label{eq:methylamino} \begin{subarray}{ll} methylamino) - 4-methyl - 5-(1-oxo-1,2-dihydro-2-naphthylidenemethyl) imidazole and 5-(1-hydroxy-2-naphthylmethyl) imidazole, resp. \end{subarray}$ 37842-56-1P RL: SPN (Synthetic preparation): PREP (Preparation)

CN 1-Naphthalenol, 2-[(5-methyl-2-[methyl(phenylmethyl)amino]-1H-imidazol-4-yl]methyl]- (9CI) (CA INDEX NAME)

(prepn. of) 37842-56-1 CAPLUS

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